

# Crystal Data Space-Group Tables

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Crystal Data Space-Group Tables lists over 17,000 materials whose space groups and symmetry have been determined mainly by x-ray diffraction. These tables comprise a companion publication to *Crystal Data Determinative Tables*. The space groups are listed in the same order and orientation as in *International Tables for x-ray Crystallography*. Within each space group, the materials are arranged in increasing order of the ratios of the cell parameters. The space-group tables enable the user to find crystals of any specified symmetry, to locate isostructural molecules, and to compare the population frequencies of the various space groups.

Key words: Crystal; isostructural materials; lattice; point group; polymorphism; space group; symmetry.

## Introduction

In recent decades, the importance of symmetry in physics, chemistry and biology has been widely recognized. Knowledge of symmetry aids theoretical studies and the interpretation and understanding of physical phenomena. In fact, it is thought that every law of physics goes back to some symmetry of nature [1].<sup>1</sup> Such information helps in the study of electronic wave functions, lattice dynamics, and point defects in crystalline lattices. Knowledge of the point-group symmetry of the molecule greatly simplifies the interpretation of molecular spectra and makes possible the identification of modes of vibration and rotation. The point-group symmetry of a molecule can frequently be determined from knowing the space group in which the compound (or a similar one) crystallizes and the number of molecules in the unit cell. Symmetry plays a vital role in the intuitive grasp of and precise mathematical description of physical properties associated with a crystal. Symmetry aids in the interpretation of elasticity, birefringence, refraction, para-, dia-, and ferro-magnetism, pyro-, piezo-, and ferro-electricity, magnetic susceptibility, polarizability, and electrical and thermal conductivity. For a detailed discussion of the structure-property relationships see Nye [2] and Newnham [3]; for an extensive mathematical treatment of symmetry see *International Encyclopedia of Physical Chemistry and Chemical Physics* [4].

The space group provides the scientist with the symmetry elements of the crystal and from these one can often deduce the symmetry of a given constituent ion or molecule. X-ray diffraction is the principal experimental tool for determining the space group of a crystal. A complete list and discussion of the 230 space groups is given in *International Tables for X-ray Crystallography* [5].

Crystal Data Space-Group Tables lists compounds according to the space group in which they crystallize. Earlier tables of compounds listed by space group [6,7] have been used by scientists in a variety of disciplines (crystallography, spectroscopy, solid state physics, materials science, mineralogy, etc.) to find compounds that may possess certain properties.

The first publication that classified crystalline materials by space group was *Systematic Tables, Part I of Crystal Data* by Werner Nowacki [6]. This publication provided scientists with a source that listed all the compounds whose space groups had been studied to that date. Nowacki also subdivided the compounds listed in each space group into categories determined by the chemical composition. In Part II of *Crystal Data*, by J. D. H. Donnay [6], crystalline substances are classified on the basis of the cell dimensions. The second edition of *Crystal Data* consists of two companion publications, *Crystal Data Determinative Tables* [8], and *Crystal Data Systematic Tables* [7]; Nowacki based *Systematic Tables on Determinative Tables* [8]. The present publication, *Crystal Data Space-Group Tables* is based on the third edition of *Determinative Tables* [9], thus following

<sup>1</sup> Figures in brackets indicate literature references.  
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a pattern now familiar to users. In the following space-group tables, the user can find isostructural materials and crystals of given symmetry. Isostructural materials can be located readily, because substances with the same space group and similar cell dimension ratios appear close to one another in these tables. Polymorphic substances can be identified by noting compounds with the same formula that crystallize in different space groups. For new materials, the space-group tables will sometimes eliminate the need for a full x-ray structure determination or will provide a short cut to the structure solution. Information gleaned from these tables may suggest or support theoretical studies on why materials crystallize in some space groups more than in others.

These space-group tables, like those of Nowacki [6, 7], make the primary classification by space group. They differ, however, because within each space group the compounds are ordered by their cell dimensions rather than by their chemistry. The introduction to the third edition of *Determinative Tables* [9] gives the types of compounds included, the literature coverage, and the rules of the determinative classification. Supplementary volumes to the third edition of *Determinative Tables* are in preparation and as they are completed, the space-group tables will be revised to include the new materials.

### Arrangement of These Space-Group Tables

The space-group tables were prepared from NBS Magnetic Tape 9<sup>2</sup> which contains data selected from each entry in the third edition of *Determinative Tables*. All those entries for which the space group is given were taken from the tape. The entries were sorted first on the space group number (1 through 230) and then on the determinative number:  $a/b$  for the trimetric crystal systems,  $c/a$  for the dimetric systems, and  $a$  for the cubic system.

The space groups are listed in the same order and expressed in the same orientation as in Volume 1 of *International Tables for X-ray Crystallography*. The following conventions are followed:

(1) For monoclinic crystals, the unique axis is labeled  $b$ . Thus crystals in space group No. 14 (which may have any of the equivalent descriptions  $P2_1/c = P2_1/a = P2_1/n$ ) are all listed under  $P2_1/c$ .

(2) Rhombohedral cells are always expressed as their hexagonal equivalents. Their determinative numbers are, therefore, the  $c/a$  ratios for the hexagonal cells.

(3) There are 22 space groups that form 11 enantiomorphic pairs. For each of the 11 pairs, all entries reported for both members of the pair are listed under the space group with the lower order number.

<sup>2</sup> For information about the tape and its lease, contact the National Technical Information Service (NTIS), Department of Commerce, 5285 Port Royal Road, Springfield, VA 22151.

These pairs are:

for the tetragonal system,

$P4_1$ No. 76	$P4_122$ No. 91	$P4_12_12$ No. 92
$P4_3$ No. 78	$P4_322$ No. 95	$P4_32_12$ No. 96

for the hexagonal system,

$P3_1$ No. 144	$P3_112$ No. 151	$P3_121$ No. 152
$P3_2$ No. 145	$P3_212$ No. 153	$P3_221$ No. 154
	$P6_1$ No. 169	
	$P6_5$ No. 170	
$P6_2$ No. 171	$P6_222$ No. 178	$P6_222$ No. 180
$P6_4$ No. 172	$P6_522$ No. 179	$P6_422$ No. 181

for the cubic system,

$P4_332$ No. 212
$P4_132$ No. 213.

The heading preceding any given space group includes: the space group in both Hermann-Mauguin and Schoenflies notations, the point group, the space-group number, and the number of inorganic and organic entries that occur in the space group. Under each space-group heading, the entries are listed in increasing order of the determinative number.

Next to the determinative number comes the chemical formula of the substance as it appears in the entry in the third edition of *Determinative Tables*. The determinative number refers the user to the complete entry in *Determinative Tables* which contains the full compound name, unit cell, literature references, and other data. Note that a *compound* may occur several times under a given space group since there are multiple entries for many compounds in the *Determinative Tables*. If the same compound appears under more than one space group, polymorphism is usually indicated. Occasionally multiple listing occurs because scientists have disagreed about the space-group assignment.

### Statistics

The space-group tables make possible the analysis of the population frequency by crystal system and by space group. The results of such an analysis are given in tables 1, 2, and 3 of this introduction. For earlier statistical analyses of the space group occurrences and their significance see *Crystal Data Systematic Tables* [7], Nowacki's early papers [10] and Nowacki, Matsumoto, and Edenharter [11], and Mackay [12]. Care must be exercised in making any statistical analyses from the present tables or in comparing them with Nowacki's earlier tables for the following reasons: (1) we did not eliminate multiple entries for compounds in our listing and counting; (2) certain groups of compounds, namely carbides,

carbonates, cyanides and cyanates occur in both the inorganic and organic lists; (3) Nowacki assumed certain space groups in cases where only a diffraction aspect was assigned in the third edition of *Crystal Data Determinative Tables* [9] (our space-group listing does not include diffraction aspects). Our tables show a great increase over Nowacki's *Systematic Tables* in some space groups of high symmetry because the third edition of *Determinative Tables* included many intermetallics which had been omitted from the second edition. In addition, statistical analyses of these data should be interpreted with caution since the numbers of compounds in various space groups are strongly influenced by the groups of compounds scientists have chosen to study. For instance, large series of certain structure types such as the garnets and pyrochlores have been synthesized and investigated. Variations in public support and in what is scientifically fashionable at different times also influence the coverage.

Taking the above precautions into account, one may still draw valid conclusions concerning those space groups with very high population frequency and those with very low. Table 3 shows, for example, that there are many space groups with few representatives and only a few space groups with many representatives. In his books on molecular crystallography, Kitaigorodsky [13, 14] has shown the prevalence of certain space groups among organic compounds, and

interpreted the reasons for this prevalence. Our tables further support his ideas. The molecular crystals of most organic compounds are rather easily represented by the packing of simple geometrical models. If all possible packings of solids of various models are examined, there are only a few space groups in which efficient packing is possible (closest packing or maximum density). Kitaigorodsky showed that for molecules without symmetry elements the following space groups provide the most efficient packing:  $P1$ ,  $P2_1$ ,  $P2_1/c$ ,  $Pca2_1$ ,  $Pna2_1$ ,  $P2_12_12_1$ . For molecules with a

TABLE 1. Population frequency by crystal system

Crystal system	Space-group numbers	Inorganic	Organic	Total
Anorthic	1-2	223	434	657
Monoclinic	3-15	1,586	2,915	4,501
Orthorhombic	16-74	2,130	1,717	3,847
Tetragonal	75-142	1,534	316	1,850
Hexagonal	143-194	2,782	369	3,151
Cubic	195-230	3,386	175	3,561
Totals		11,641	5,926	17,567

TABLE 2. Frequency for closest packed and maximum density space groups for organic crystals <sup>a</sup>

Molecular symmetry <sup>b</sup>	Space group	Number of entries <sup>c</sup>	Percent of total organic entries <sup>d</sup>	Percent of organic entries in crystal system
1	$P1$	57	1	13
	$P2_1$	458	8	16
	$Pca2_1$	44	1	3
	$Pna2_1$	100	2	6
	$P2_12_12_1$	722	12	42
	$P2_1/c$	1783	30	61
$\bar{1}$	$P\bar{1}$	377	6	87
	$Pbca$	210	4	12
	$C2/c$	315	5	11
2	$P2_12_12$	104	2	6
	$Pbcn$	65	1	4
m	$Pmc2_1$	4	0.07	0.2
	$Cmc2_1$	9	0.15	0.5
	$Pnma$	124	2	7
		4372	74%	

<sup>a</sup> See Kitaigorodsky [13] for detailed discussion.

<sup>b</sup> Molecules with the specified symmetry element(s) can pack efficiently in the indicated space groups.

<sup>c</sup> Number of entries in the space-group tables.

<sup>d</sup> Note that:

30 percent of all organic entries are in  $P2_1/c$ .

65 percent of all organic entries are in  $P\bar{1}$ ,  $P2_1$ ,  $P2_1/c$ ,  $C2/c$ ,  $P2_12_12_1$ ,  $Pbca$ .

87 percent of all monoclinic entries are in 3 space groups,  $P2_1$ ,  $P2_1/c$ ,  $C2/c$ .

54 percent of all orthorhombic entries are in 2 space groups,  $P2_12_12_1$ ,  $Pbca$ .

TABLE 3. Space group frequency

Many space groups have only a few representatives; a few space groups have many representatives.

Inorganic		Organic	
No. of space groups <sup>b</sup>	No. of compounds in each space group	No. of space groups <sup>b</sup>	No. of compounds in each space group
1 ( <i>Fm3m</i> )	991	1 ( <i>P2<sub>1</sub>/c</i> )	1783
1 ( <i>Pnma</i> )	794	1 ( <i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i> )	722
1 ( <i>Fd3m</i> )	651	1 ( <i>P2<sub>1</sub></i> )	458
1 ( <i>P6<sub>3</sub>/mmc</i> )	637	1 ( <i>P1</i> )	377
1 ( <i>P2<sub>1</sub>/c</i> )	588	1 ( <i>C2/c</i> )	315
1 ( <i>Pm3m</i> )	573	1 ( <i>Pbca</i> )	210
1 ( <i>R3m</i> )	451	1 ( <i>Pnma</i> )	124
1 ( <i>C2/m</i> )	310	1 ( <i>P2<sub>1</sub>2<sub>1</sub>2</i> )	104
1 ( <i>C2/c</i> )	301	1 ( <i>Pna2<sub>1</sub></i> )	100
1 ( <i>Cmcm</i> )	258	1 ( <i>C2</i> )	80
1 ( <i>R3</i> )	226	1 ( <i>P2<sub>1</sub>/m</i> )	77
1 ( <i>P3m1</i> )	225	1 ( <i>Fm3m</i> )	66
1 ( <i>P6/mmm</i> )	220	1 ( <i>Pbcn</i> )	65
1 ( <i>I4/mmm</i> )	215	1 ( <i>P1</i> )	57
1 ( <i>P1</i> )	207	1 ( <i>Cc</i> )	50
12	101-200	1 ( <i>R3</i> )	50
11	61-100	9	31-50
15	41-60	16	16-30
19	26-40	22	9-15
21	17-25	19	5-8
25	10-16	20	4
31	5-9	17	3
30	3-4	18	2
22	1-2	27	1
18	0	55	0

<sup>a</sup> There are 17,567 compounds (whose space groups have been determined) in the 3rd edition of Crystal Data. 11,641 are classified as inorganic; 5,926 as organic.

<sup>b</sup> Total=219 (11 enantiomorphic pairs).

<sup>c</sup> Note that 137 space groups for the organic compounds have 4 or fewer compounds; for the inorganic 101 have 9 or fewer representatives.

center of symmetry, the space groups are: *P1*, *P2<sub>1</sub>/c*, *C2/c*, *Pbca*; for a 2-fold axis, *C2/c*, *P2<sub>1</sub>2<sub>1</sub>2*, *Pbcn*; for a mirror plane, *Pmc2<sub>1</sub>*, *Cmc2<sub>1</sub>*, *Pnma*. Table 2 gives the frequency of the above space groups in our compilation. As suggested by earlier data, these are indeed (with a couple of exceptions) very common space groups.

The fact that the majority of organic molecules fall in the first three crystal systems and in a relatively few space groups is explained, then, by the simple packing arguments outlined by Kitaigorodsky. The situation is more complex for the inorganic materials because of the diversity of materials and the variety of bonding types (see Wells [15]). Table 1 shows that the inorganic crystal systems are much more evenly populated than the organic. Nevertheless, we again note a concentration within a few space groups. For the cubic system, two-thirds of the compounds are described in *Fd3m* (pyrochlore type and derivative structures), *Fm3m* (NaCl type and derivative structures), and *Pm3m* (CsCl type, simple perovskite type, and their derivative structures). Similarly, for the hexagonal system, more than one-third of the compounds crystallize in *P6<sub>3</sub>/mmc* (a variety of intermetallic structure types) and *R3m* (apatite type, and intermetallic structure types).

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1	P1 C <sub>1</sub> <sup>1</sup>	No. 1	Inorganic - 16 Organic - 57
Inorganic			
0.3707	(Mg, Fe, Al) <sub>6</sub> (OH) <sub>8</sub> (Si, Al) <sub>4</sub> O <sub>10</sub>	0.7855	Pr(N <sub>2</sub> O) <sub>3</sub> ·6H <sub>2</sub> O
0.3726	AlMg <sub>5</sub> (OH) <sub>8</sub> (Si, Al) <sub>4</sub> O <sub>10</sub>	0.8155	Al <sub>2</sub> (OH) <sub>4</sub> Si <sub>2</sub> O <sub>5</sub>
0.3772	Ca <sub>2</sub> (VO) <sub>4</sub> (V <sub>2</sub> O <sub>7</sub> ) <sub>3</sub> ·7H <sub>2</sub> O	0.8326	Na <sub>2</sub> Al(OH)Si <sub>3</sub> O <sub>8</sub>
0.4246	FeFe <sub>2</sub> (SO <sub>4</sub> ) <sub>4</sub> ·14H <sub>2</sub> O	0.8387	Ti <sub>5</sub> O <sub>9</sub>
0.5045	Ca <sub>8</sub> Cl <sub>4</sub> (B <sub>6</sub> O <sub>11</sub> ) <sub>3</sub> ·4H <sub>2</sub> O	0.8699	ZnMoO <sub>4</sub>
0.5466	Ce <sub>2</sub> Tl(Si, P)(O, OH) <sub>7</sub> ·4H <sub>2</sub> O	0.9428	(Fe, Mg) <sub>3</sub> (Si, Al) <sub>4</sub> O <sub>10</sub> (OH) <sub>5</sub>
0.6966	Fe <sub>2</sub> Mn(OH) <sub>2</sub> (PO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O	0.9805	(Ca, Sr) <sub>2</sub> [B <sub>5</sub> O <sub>8</sub> (OH) <sub>2</sub> Cl]
0.7533	RbBe <sub>2</sub> F <sub>5</sub>	0.9870	PtCrO <sub>4</sub> ·H <sub>2</sub> O
Organic			
0.1263	C <sub>19</sub> H <sub>36</sub> O <sub>2</sub>	0.7195	C <sub>9</sub> H <sub>11</sub> BrN <sub>2</sub> O <sub>5</sub>
0.1768	C <sub>12</sub> H <sub>25</sub> ·NH <sub>2</sub> CH <sub>3</sub> Cl	0.7248	C <sub>11</sub> H <sub>17</sub> ON
0.1842	C <sub>27</sub> H <sub>45</sub> OH·H <sub>2</sub> O	0.7392	C <sub>9</sub> H <sub>11</sub> IN <sub>2</sub> O <sub>5</sub>
0.2658	C <sub>19</sub> H <sub>30</sub> OH-CH(CH <sub>3</sub> )(CH <sub>2</sub> ) <sub>2</sub> CH(C <sub>2</sub> H <sub>5</sub> )CH(CH <sub>3</sub> ) <sub>2</sub> ·2H <sub>2</sub> O	0.7477	C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> AuCl <sub>4</sub>
0.2666	C <sub>19</sub> H <sub>30</sub> OH-CH(CH <sub>3</sub> )(CH <sub>2</sub> ) <sub>2</sub> CH(C <sub>2</sub> H <sub>5</sub> )CH(CH <sub>3</sub> ) <sub>2</sub> ·2H <sub>2</sub> O	0.7491	C <sub>11</sub> H <sub>14</sub> O <sub>6</sub>
0.2782	C <sub>19</sub> H <sub>30</sub> OH-CH(CH <sub>3</sub> )(CH <sub>2</sub> ) <sub>3</sub> CH(CH <sub>3</sub> ) <sub>2</sub> ·2H <sub>2</sub> O	0.7603	C <sub>21</sub> H <sub>36</sub> O <sub>2</sub>
0.2784	C <sub>19</sub> H <sub>28</sub> OH-CH(CH <sub>3</sub> )(CH <sub>2</sub> ) <sub>2</sub> CH(C <sub>2</sub> H <sub>5</sub> )CH(CH <sub>3</sub> ) <sub>2</sub> ·2H <sub>2</sub> O	0.7732	C <sub>34</sub> H <sub>50</sub> O <sub>3</sub>
0.2991	C <sub>19</sub> H <sub>30</sub> OH-CH(CH <sub>3</sub> )(CH <sub>2</sub> ) <sub>3</sub> CH(CH <sub>3</sub> ) <sub>2</sub>	0.7888	(C <sub>19</sub> H <sub>30</sub> O <sub>2</sub> ) <sub>2</sub> ·C <sub>6</sub> H <sub>5</sub> OHBr
0.3032	C <sub>19</sub> H <sub>30</sub> OH-CH(CH <sub>3</sub> )(CH <sub>2</sub> ) <sub>2</sub> CH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>	0.7893	C <sub>44</sub> H <sub>28</sub> N <sub>4</sub> Zn
0.3157	C <sub>21</sub> H <sub>42</sub> O <sub>4</sub>	0.8002	Cd[SC(CH <sub>3</sub> )NH <sub>2</sub> ] <sub>2</sub> (NCS) <sub>2</sub>
0.3506	C <sub>27</sub> H <sub>45</sub> OH·CH <sub>3</sub> OH	0.8159	NaB <sub>10</sub> H <sub>13</sub> O(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O
0.3688	C <sub>27</sub> H <sub>45</sub> OH·H <sub>2</sub> O	0.8584	C <sub>19</sub> H <sub>30</sub> O <sub>2</sub> ·C <sub>6</sub> H <sub>5</sub> OHBr
0.3831	C <sub>6</sub> H <sub>13</sub> N <sub>2</sub> O	0.8667	(CH <sub>3</sub> ) <sub>2</sub> CH·CH <sub>2</sub> ·CH(NH <sub>2</sub> )CO·NH·CH <sub>2</sub> -COOH·2H <sub>2</sub> O
0.4153	C <sub>27</sub> H <sub>45</sub> OH	0.8732	C <sub>28</sub> H <sub>42</sub> O <sub>7</sub>
0.4166	C <sub>12</sub> H <sub>17</sub> BrN <sub>2</sub> O <sub>5</sub>	0.8744	UO <sub>2</sub> (C <sub>6</sub> H <sub>4</sub> OHCOO) <sub>2</sub> ·2H <sub>2</sub> O
0.4640	C <sub>15</sub> H <sub>14</sub> O <sub>2</sub>	0.8796	(C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> NHCr <sub>2</sub> (CO) <sub>10</sub>
0.4695	C <sub>27</sub> H <sub>48</sub> O <sub>2</sub> ·2H <sub>2</sub> O	0.8925	C <sub>19</sub> H <sub>26</sub> O <sub>2</sub> ·C <sub>6</sub> H <sub>5</sub> OHBr
0.4848	C <sub>29</sub> H <sub>40</sub> BrN <sub>2</sub> O <sub>11</sub> S·H <sub>2</sub> O	0.9223	C <sub>19</sub> H <sub>22</sub> O <sub>2</sub> ·H <sub>2</sub> SO <sub>4</sub> ·8H <sub>2</sub> O
0.5152	(C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> Cu(N <sub>2</sub> O) <sub>2</sub> ·2H <sub>2</sub> O	0.9272	(C <sub>2</sub> H <sub>5</sub> ) <sub>6</sub> B <sub>3</sub> N <sub>3</sub>
0.5332	C <sub>27</sub> H <sub>46</sub> O <sub>2</sub>	0.9364	C <sub>12</sub> H <sub>28</sub> Si <sub>4</sub>
0.5421	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub> S	0.9551	C <sub>19</sub> H <sub>30</sub> O <sub>2</sub> ·C <sub>6</sub> H <sub>5</sub> OHBr
0.5683	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>	0.9569	P <sub>4</sub> N <sub>4</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> (NHCH <sub>3</sub> ) <sub>4</sub>
0.5941	C <sub>5</sub> H <sub>9</sub> N <sub>3</sub> ·2HBr	0.9572	C <sub>21</sub> H <sub>18</sub> N <sub>8</sub> O <sub>14</sub>
0.6070	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub> ·HBr·H <sub>2</sub> O	0.9669	C <sub>38</sub> H <sub>58</sub> O <sub>9</sub> N <sub>8</sub> ·4H <sub>2</sub> O
0.6236	Na[CKN <sub>2</sub> O] <sub>2</sub>	0.9824	(C <sub>9</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> ) <sub>2</sub> C <sub>20</sub> H <sub>12</sub>
0.6379	C <sub>4</sub> NH <sub>8</sub> COOH	0.9859	(CH <sub>3</sub> ) <sub>2</sub> N·C <sub>6</sub> H <sub>4</sub> ·NCS
0.6667	(C <sub>19</sub> H <sub>22</sub> O <sub>2</sub> ) <sub>2</sub> ·H <sub>2</sub> SO <sub>4</sub> ·2H <sub>2</sub> O	0.9878	C <sub>6</sub> H <sub>4</sub> S <sub>4</sub> C <sub>6</sub> H <sub>4</sub>
0.6963	C <sub>7</sub> H <sub>10</sub> O <sub>7</sub> ·H <sub>2</sub> O	0.9998	C <sub>19</sub> H <sub>30</sub> O <sub>2</sub> ·C <sub>6</sub> H <sub>5</sub> OHBr
0.6993	C <sub>14</sub> H <sub>12</sub> O <sub>7</sub>		

1	P1 C <sub>1</sub> <sup>1</sup>	No. 2	Inorganic - 207 Organic - 377
Inorganic			
0.0221	KR <sub>3</sub> (OH, F) <sub>2</sub> (Al, Si) <sub>4</sub> O <sub>10</sub>	0.6545	Mn <sub>2</sub> B <sub>2</sub> O <sub>5</sub>
0.0883	KR <sub>3</sub> (OH, F) <sub>2</sub> (Al, Si) <sub>4</sub> O <sub>10</sub>	0.6574	Fe <sub>2</sub> B <sub>2</sub> O <sub>5</sub>
0.1839	Pb <sub>3</sub> As <sub>4</sub> S <sub>9</sub>	0.6637	Co <sub>2</sub> B <sub>2</sub> O <sub>5</sub>
0.3663	Pb <sub>3</sub> As <sub>4</sub> S <sub>9</sub>	0.6711	Mg <sub>2</sub> B <sub>2</sub> O <sub>5</sub>
0.3689	Pb <sub>5</sub> Sn <sub>3</sub> Sb <sub>2</sub> S <sub>14</sub>	0.6774	K <sub>4</sub> H <sub>2</sub> I <sub>2</sub> O <sub>10</sub> ·8H <sub>2</sub> O
0.3699	Mg <sub>5</sub> (Fe, Cr, Al)(Si, Al) <sub>4</sub> O <sub>10</sub> H <sub>8</sub>	0.6793	Al <sub>2</sub> Fe(OH) <sub>2</sub> (PO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O
0.3748	P <sub>4</sub> S <sub>3</sub> I <sub>2</sub>	0.6804	Pb <sub>2</sub> (UO <sub>2</sub> )(AsO <sub>4</sub> ) <sub>2</sub>
0.4047	(Zn, Fe, Ca, Mn)Fe <sub>4</sub> (SO <sub>4</sub> ) <sub>6</sub> (OH) <sub>2</sub> ·18H <sub>2</sub> O	0.6806	I <sub>2</sub> Cl <sub>6</sub>
0.4397	Zn <sub>2</sub> (OH)PO <sub>4</sub>	0.6825	CuSO <sub>4</sub> ·H <sub>2</sub> O
0.4727	(Fe, Mn, Ca, Mg)Si <sub>2</sub> O <sub>3</sub>	0.6830	Bi <sub>4</sub> (UO <sub>2</sub> ) <sub>4</sub> (AsO <sub>4</sub> ) <sub>2</sub> ·3H <sub>2</sub> O
0.4759	Ba <sub>2</sub> Mn <sub>2</sub> (Ti, Fe)(Si <sub>2</sub> O <sub>7</sub> )(P, S) <sub>4</sub> OH	0.6840	Al <sub>2</sub> Mg(OH) <sub>2</sub> (PO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O
0.4775	(Ba, Sr, Na) <sub>2</sub> (Mn, Fe, Ca, Mg) <sub>2</sub> (Ti, Fe, Al)(Si <sub>2</sub> O <sub>7</sub> ) [(P, S) <sub>4</sub> ](OH)	0.6850	CaNaB <sub>5</sub> O <sub>9</sub> ·8H <sub>2</sub> O
0.5052	Ca <sub>4</sub> H(PO <sub>4</sub> ) <sub>3</sub> ·2H <sub>2</sub> O	0.6544	Na <sub>4</sub> P <sub>4</sub> O <sub>12</sub> ·4H <sub>2</sub> O
0.5194	Ca <sub>2</sub> KH <sub>7</sub> (PO <sub>4</sub> ) <sub>4</sub> ·2H <sub>2</sub> O	0.7074	Al <sub>2</sub> Fe(O, OH)(PO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O
0.5265	Ca(H <sub>2</sub> PO <sub>4</sub> ) <sub>2</sub> ·H <sub>2</sub> O	0.7190	Mg <sub>3</sub> (NH <sub>4</sub> ) <sub>2</sub> H <sub>4</sub> (PO <sub>4</sub> ) <sub>4</sub> ·8H <sub>2</sub> O
0.5561	K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>	0.7316	NaClO <sub>2</sub> ·3H <sub>2</sub> O
0.5606	Na <sub>10</sub> H <sub>10</sub> (W <sub>12</sub> O <sub>46</sub> )·23H <sub>2</sub> O	0.7366	(Mg, Zn) <sub>2</sub> (Na, K)H(AsO <sub>4</sub> ) <sub>2</sub> ·4H <sub>2</sub> O
0.5707	CuSO <sub>4</sub> ·5H <sub>2</sub> O	0.7371	K <sub>6</sub> (P <sub>2</sub> W <sub>18</sub> O <sub>62</sub> )·14H <sub>2</sub> O
0.5720	CuSO <sub>4</sub> ·5H <sub>2</sub> O	0.7372	ALLi(OH, F)PO <sub>4</sub>
0.5735	CuSeO <sub>4</sub> ·5H <sub>2</sub> O	0.7382	ALLi(OH, F)PO <sub>4</sub>
0.5738	Rb <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>	0.7386	Ho(ReO <sub>4</sub> ) <sub>3</sub> ·4H <sub>2</sub> O
0.5817	Al(OH) <sub>3</sub>	0.7400	ALLi(OH, F)PO <sub>4</sub>
0.6048	Mo <sub>9</sub> O <sub>26</sub>	0.7460	CaB <sub>3</sub> O <sub>3</sub> (OH) <sub>5</sub> ·2H <sub>2</sub> O
0.6415	Ca <sub>2</sub> FeFe(OH)Si <sub>5</sub> O <sub>14</sub>	0.7487	Zr(OH) <sub>2</sub> (NO <sub>3</sub> ) <sub>2</sub> ·4H <sub>2</sub> O
0.6452	Na <sub>5</sub> H <sub>3</sub> (CO <sub>3</sub> ) <sub>4</sub>	0.7517	NaB(OH) <sub>4</sub> ·2H <sub>2</sub> O
0.6500	Mn <sub>4</sub> CaSi <sub>5</sub> O <sub>15</sub>	0.7556	Co <sub>2</sub> Si(W <sub>3</sub> O <sub>10</sub> ) <sub>4</sub> ·18H <sub>2</sub> O
		0.7598	Ni <sub>2</sub> Si(W <sub>3</sub> O <sub>10</sub> ) <sub>4</sub> ·18H <sub>2</sub> O

$P\bar{1}$   $C_1^1$  No. 2 (continued)

## Inorganic (continued)

0.7638	$Zn_3(P\bar{O}_4)_2 \cdot 4H_2O$	0.9412	$Ag(Sb, Bi)_2S_2$
0.7669	$CuH_2(U\bar{O}_2Si\bar{O}_4)_2 \cdot 5H_2O$	0.9419	$FeKS_3\bar{O}_8$
0.7698	$Al_6Cu(\bar{O}H)_8(P\bar{O}_4)_4 \cdot 4H_2O$	0.9456	$K_3Re\bar{O}_2(CN)_4$
0.7702	$Cs_2S_5 \cdot H_2O$	0.9508	$Na_5P_3\bar{O}_{10} \cdot 6H_2O$
0.7714	$[(NH_3)_4Co(\bar{O}H)_2Co(NH_3)_4]Cl_4 \cdot 4H_2O$	0.9575	$HgK$
0.7724	$Al_6Cu(\bar{O}H)_8(P\bar{O}_4)_4 \cdot 5H_2O$	0.9579	$Sb_2S_2\bar{O}$
0.7741	$CuFe_6(P\bar{O}_4)_4(\bar{O}H)_8 \cdot 4H_2O$	0.9595	$FeH(SiW_{12}\bar{O}_{40}) \cdot 20H_2O$
0.7763	$RbMnCl_3 \cdot 2H_2O$	0.9620	$N\bar{O}_2HS_2\bar{O}_7$
0.7768	$CuU\bar{O}_4 \cdot 2H_2O$	0.9620	$Ag_3(N\bar{O}_3)_2SCN$
0.7780	$K_2Ca_2Mg(S\bar{O}_4)_4 \cdot 2H_2O$	0.9621	$NaI \cdot 2H_2O$
0.7789	$[(NH_3)_4Co]_2(\bar{O}H)_2Cl_4 \cdot 4H_2O$	0.9623	$[KAlSi_3\bar{O}_8]$
0.7799	$CuZn_2(As\bar{O}_4)_2$	0.9635	$NaAlSi_3\bar{O}_8$
0.7833	$Sm(N\bar{O}_3)_3 \cdot 6H_2O$	0.9637	$KAlSi_3\bar{O}_8$
0.7840	$H_5As_3\bar{O}_{10}$	0.9637	$NaAlSi_3\bar{O}_8$
0.7857	$Al_2Fe(\bar{O}H)_2(P\bar{O}_4)_2 \cdot 7H_2O$	0.9644	$NaAlSi_3\bar{O}_8$
0.7906	$K_2S_2\bar{O}_8$	0.9651	$Ni_2Si(Mo_3\bar{O}_{10})_4 \cdot 18H_2O$
0.7909	$K_4P_3\bar{O}_9NH_2 \cdot 4H_2O$	0.9661	$MnF_2$
0.7923	$CaB_3\bar{O}_3(\bar{O}H)_5 \cdot H_2O$	0.9664	$CsFe_4(N\bar{O})_7S_3 \cdot H_2O$
0.7940	$CaB_3\bar{O}_3(\bar{O}H)_5 \cdot H_2O$	0.9670	$K_2Zn_2V_{10}\bar{O}_{28} \cdot 16H_2O$
0.7962	$Cs_2S_6$	0.9681	$NaBSi_3\bar{O}_8$
0.8212	$Ce(N\bar{O}_3)_3 \cdot 6H_2O$	0.9683	$Zn_2Si(W_3\bar{O}_{10})_4 \cdot 18H_2O$
0.8225	$Fe_2Na_2K_2(Si_4\bar{O}_{10})_2 \cdot H_2O$	0.9687	$Na_4Ni(NCS)_6 \cdot 12H_2O$
0.8265	$Mg_2(\bar{O}H)_3Br \cdot 4H_2O$	0.9688	$K_2Re_2Cl_8 \cdot 2H_2O$
0.8332	$La(N\bar{O}_3)_3 \cdot 6H_2O$	0.9689	$[NaAlSi_3\bar{O}_8]$
0.8360	$Fe_3(As\bar{O}_4)_2 \cdot 8H_2O$	0.9691	$NaBSi_3\bar{O}_8$
0.8390	$Ca_2Mg(As\bar{O}_4)_2 \cdot 2H_2O$	0.9704	$Pt(NH_3)_2Cl_2$
0.8430	$Ca_2Fe(P\bar{O}_4)_2 \cdot 4H_2O$	0.9706	$KFe_4(N\bar{O})_7S_3 \cdot H_2O$
0.8469	$Ag_3P_3\bar{O}_9 \cdot H_2O$	0.9715	$K_2ZrSi_6\bar{O}_{15}$
0.8482	$Ca_2(Mg, Fe)(P\bar{O}_4)_2 \cdot 2H_2O$	0.9728	$NaBSi_3\bar{O}_8$
0.8484	$K_6V_{10}\bar{O}_{28} \cdot 10H_2O$	0.9733	$W\bar{O}_3$
0.8538	$BaTe(S_2\bar{O}_3)_2 \cdot 2H_2O$	0.9756	$(K, Na)_2(Fe, Mn)_7Ti_2(Si_4\bar{O}_{12})_2(\bar{O}, \bar{O}H)_3(\bar{O}H, F)_4$
0.8559	$K_2W_2\bar{O}_{11} \cdot 4H_2O$	0.9761	$Mg_9B_2\bar{O}_{12} \cdot 8H_2O$
0.8590	$Mg_2(\bar{O}H)_3Cl \cdot 4H_2O$	0.9779	$W\bar{O}_3$
0.8690	$Na_4NiW_6\bar{O}_{24}H_6 \cdot 16H_2O$	0.9780	$(K, Na)AlSi_3\bar{O}_8$
0.8711	$Zn_2(\bar{O}H)(As\bar{O}_4)$	0.9786	$Al_2BCa_2(Fe_{0.7}Mn_{0.3})HSi_4\bar{O}_{16}$
0.8742	$(Pb, Tl)_2AgAs_2S_5$	0.9809	$CaAl_2Si_2\bar{O}_8$
0.8746	$Zn_2(\bar{O}H)P\bar{O}_4$	0.9813	$Cu(NH_3)_4(CuI_2)_2$
0.8768	$ZrF_4 \cdot 3H_2O$	0.9818	$K_2Mg_2V_{10}\bar{O}_{28} \cdot 16H_2O$
0.8795	$Zn_2(\bar{O}H)P\bar{O}_4$	0.9841	$(K, Na)_3(Fe, Mn)_7Ti_2Si_8(\bar{O}, \bar{O}H, F)_{31}$
0.8796	$Ca_2(Mn, Fe)(P\bar{O}_4)_2 \cdot 2H_2O$	0.9856	$Ga_2Cl_6$
0.8804	$[Pt(NH_3)_3Cl_3]Cl \cdot H_2O$	0.9857	$CaHP\bar{O}_4$
0.8811	$Ca_2NaHSi_3\bar{O}_9$	0.9860	$KAlSi_3\bar{O}_8$
0.8828	$Ca_2(Mn, Fe)(P\bar{O}_4)_2 \cdot 2H_2O$	0.9866	$H_5BW_{12}\bar{O}_{40} \cdot 14H_2O$
0.8881	$Ca_2P_2\bar{O}_7 \cdot 2H_2O$	0.9870	$(K, Na)AlSi_3\bar{O}_8$
0.8885	$(Na, Ca, Mn)_3(Fe, Ti, Zr)FSi_2\bar{O}_8$	0.9873	$(K, Na)AlSi_3\bar{O}_8$
0.8894	$Ca_2(Fe, Mn)(P\bar{O}_4)_2 \cdot 2H_2O$	0.9874	$3Cu(I\bar{O}_3)_2 \cdot 2H_2O$
0.8901	$LaCl_3 \cdot nH_2O$	0.9883	$Ca(V\bar{O}_3)_2 \cdot 4H_2O$
0.8912	$Na_3P_3\bar{O}_9 \cdot 6H_2O$	0.9897	$(KPhCl_3)_3 \cdot H_2O$
0.8922	$Pd(NH_3)_2(N\bar{O}_2)_2$	0.9906	$K_4[Th(S\bar{O}_4)_4(H_2\bar{O})_2]$
0.8953	$NaP\bar{O}_3$	0.9909	$H_4SiW_{12}\bar{O}_{40} \cdot 14H_2O$
0.8985	$BaS(S_2\bar{O}_3)_2 \cdot 2H_2O$	0.9915	$Na_{1-x}Ca_xAl_{1+x}Si_{3-x}\bar{O}_8$
0.9005	$Al_2Ge\bar{O}_5$	0.9923	$Ca[B(\bar{O}H)_4]_2$
0.9029	$Na_3P_3\bar{O}_9 \cdot 6H_2O$	0.9926	$Cs_2Mg_2V_{10}\bar{O}_{28} \cdot 16H_2O$
0.9053	$Fe_2Ge\bar{O}_5$	0.9930	$H_4SiMo_{12}\bar{O}_{40} \cdot 14H_2O$
0.9072	$Al_2Si\bar{O}_5$	0.9937	$H_3PMo_{12}\bar{O}_{40} \cdot 14H_2O$
0.9082	$Cd_2Si(Mo_3\bar{O}_{10})_4 \cdot 22H_2O$	0.9938	$[CaAl_2Si_2\bar{O}_8]$
0.9094	$Ca(V\bar{O}_3)_2 \cdot 2H_2O$	0.9942	$Na_{0.34}K_{0.01}Ca_{0.65}Al_{1.65}Si_{2.35}\bar{O}_8$
0.9111	$PrCl_3 \cdot nH_2O$	0.9944	$CaHAs\bar{O}_4$
0.9161	$Cs_2MnCl_4 \cdot 2H_2O$	0.9955	$NaAlSi_3\bar{O}_8$
0.9173	$ZnMn_3\bar{O}_7 \cdot 3H_2O$	0.9956	$(Na, K, Ca)(Si, Al)_4\bar{O}_8$
0.9184	$Al_2Si\bar{O}_5$	0.9959	$Al_3Si_2(\bar{O}H)_3\bar{O}_7$
0.9210	$Na_2H(P\bar{O}_3)_3$	0.9960	$P_4S_{10}$
0.9216	$Cd_2Si(W_3\bar{O}_{10})_4 \cdot 23H_2O$	0.9964	$K_{0.157}Na_{0.742}Ca_{0.101}(Al_{1.101}Si_{2.899}\bar{O}_8)$
0.9216	$Mn_2Si(W_3\bar{O}_{10})_4 \cdot 22H_2O$	0.9965	$(Na, K, Ca)(Si, Al)_4\bar{O}_8$
0.9219	$NaAs\bar{O}_3$	0.9969	$(NH_4)_4Mo_8\bar{O}_{26} \cdot 5H_2O$
0.9244	$Rb_2MnCl_4 \cdot 2H_2O$	0.9972	$(Na, K, Ca)(Si, Al)_4\bar{O}_8$
0.9275	$Na_2Si\bar{O}_3 \cdot 5H_2O$	0.9975	$CaMnSi_2\bar{O}_6$
0.9282	$(Ca, Na)Al_2Si_2\bar{O}_8$	0.9976	$Ca(AlSi\bar{O}_4)_2$
0.9288	$Na_2H_2Si\bar{O}_4 \cdot 4H_2O$	0.9976	$(Na, K, Ca)(Si, Al)_4\bar{O}_8$
0.9301	$CdCu_3(\bar{O}H)_6(N\bar{O}_3)_2 \cdot 2H_2O$	0.9980	$H_3B\bar{O}_3$
0.9317	$Ca_2Fe(P\bar{O}_4)_2 \cdot 4H_2O$	0.9983	$(Na, K, Ca)(Si, Al)_4\bar{O}_8$
0.9348	$(NH_4)_2Mo_2\bar{O}_7$	0.9986	$CaC_2$
0.9370	$Pb_7Sb_{12}S_{25}$	0.9986	$(Na, Ca, K)(Si, Al)_4\bar{O}_8$
0.9371	$[Pt(NH_3)_6]Cl_4 \cdot H_2O$	0.9986	$H_3PW_{12}\bar{O}_{40} \cdot 14H_2O$

PI C<sub>1</sub><sup>1</sup> No. 2 (continued)

## Inorganic (continued)

0.9987	(Mn, Ca)Si <sub>3</sub> O <sub>8</sub>	1.0000	(Na, Ca, K)(Si, Al) <sub>4</sub> O <sub>8</sub>
0.9992	(Na, Ca, K)(Si, Al) <sub>4</sub> O <sub>8</sub>	1.0000	(K, Na)AlSi <sub>3</sub> O <sub>8</sub>
1.0000	(NH <sub>4</sub> ) <sub>6</sub> [(CrO) <sub>2</sub> (Mo <sub>3</sub> O <sub>10</sub> ) <sub>4</sub> ] <sub>2</sub> ·2OH <sub>2</sub> O	1.0000	(Na, Ca)Al(Si, Al) <sub>3</sub> O <sub>8</sub>

## Organic

0.1168	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>7</sub> CH=CH(CH <sub>2</sub> ) <sub>11</sub> C <sub>6</sub> H <sub>5</sub>	0.6183	Te[(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> PS <sub>2</sub> ] <sub>2</sub>
0.1270	C <sub>14</sub> H <sub>29</sub> C <sub>6</sub> H <sub>5</sub>	0.6220	C <sub>18</sub> H <sub>12</sub>
0.1481	C <sub>15</sub> H <sub>31</sub> C <sub>6</sub> H <sub>5</sub>	0.6235	N <sub>6</sub> C <sub>6</sub> H <sub>4</sub> ·CH:CH·C <sub>6</sub> H <sub>5</sub>
0.1552	C <sub>19</sub> H <sub>38</sub> O <sub>2</sub>	0.6264	[(CH <sub>3</sub> ) <sub>2</sub> AsS] <sub>2</sub>
0.1626	C <sub>18</sub> H <sub>30</sub> O <sub>2</sub>	0.6292	C <sub>17</sub> H <sub>24</sub> O <sub>2</sub>
0.1671	C <sub>19</sub> H <sub>38</sub> O <sub>2</sub>	0.6303	(CH <sub>4</sub> N <sub>2</sub> ) <sub>2</sub> ·C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>
0.1705	[CH <sub>3</sub> (CH <sub>2</sub> ) <sub>10</sub> C <sub>6</sub> H <sub>5</sub> ] <sub>2</sub>	0.6317	(CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> ·2H <sub>2</sub> O
0.1723	C <sub>15</sub> H <sub>31</sub> C <sub>6</sub> H <sub>5</sub>	0.6336	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
0.1739	[Br(CH <sub>2</sub> ) <sub>10</sub> C <sub>6</sub> H <sub>5</sub> ] <sub>2</sub>	0.6348	C <sub>18</sub> H <sub>16</sub> O <sub>4</sub>
0.1752	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>8</sub> SC <sub>2</sub> H <sub>5</sub>	0.6367	C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
0.1768	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> CHBrCH <sub>2</sub> C <sub>6</sub> H <sub>5</sub>	0.6376	C <sub>3</sub> H <sub>4</sub> O <sub>4</sub>
0.1876	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	0.6377	Cl·C <sub>6</sub> H <sub>4</sub> ·S <sub>2</sub> ·CH <sub>3</sub>
0.2089	C <sub>18</sub> H <sub>38</sub>	0.6397	CaC <sub>8</sub> H <sub>6</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ·2H <sub>2</sub> O
0.2243	C <sub>14</sub> H <sub>29</sub> C <sub>6</sub> H <sub>5</sub>	0.6400	Te(CSN <sub>2</sub> H <sub>4</sub> ) <sub>4</sub> (HF <sub>2</sub> ) <sub>2</sub>
0.2314	(Cl·CH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> ·NCS	0.6409	C <sub>12</sub> H <sub>20</sub> O <sub>4</sub>
0.2316	C <sub>23</sub> H <sub>46</sub> O <sub>2</sub> NBr	0.6441	Te(C <sub>2</sub> H <sub>5</sub> N <sub>2</sub> S) <sub>4</sub> Br <sub>2</sub>
0.2395	C <sub>19</sub> H <sub>38</sub> O <sub>2</sub>	0.6452	Na <sub>5</sub> H <sub>3</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub>
0.2468	CH <sub>3</sub> C <sub>17</sub> H <sub>34</sub> C <sub>6</sub> H <sub>5</sub>	0.6492	(NH <sub>2</sub> CSNH <sub>2</sub> ) <sub>4</sub> TeCl <sub>2</sub>
0.2502	C <sub>23</sub> H <sub>46</sub> O <sub>2</sub> NI	0.6512	C <sub>36</sub> H <sub>60</sub> O <sub>12</sub> N <sub>4</sub>
0.2604	CH <sub>3</sub> C <sub>17</sub> H <sub>34</sub> C <sub>6</sub> H <sub>5</sub>	0.6641	C <sub>5</sub> H <sub>4</sub> O <sub>3</sub>
0.2613	C <sub>2</sub> H <sub>5</sub> C <sub>15</sub> H <sub>30</sub> C <sub>6</sub> H <sub>5</sub>	0.6651	KH(C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>2</sub>
0.2688	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub> NI	0.6651	K(HC <sub>2</sub> H <sub>4</sub> )(H <sub>2</sub> C <sub>2</sub> H <sub>4</sub> )·2H <sub>2</sub> O
0.2919	C <sub>21</sub> H <sub>44</sub> O <sub>2</sub> NI	0.6697	C <sub>6</sub> H <sub>5</sub> ·C <sub>6</sub> H <sub>3</sub> ClC <sub>6</sub> H <sub>5</sub>
0.3101	Sr(C <sub>7</sub> H <sub>15</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ·xH <sub>2</sub> O	0.6735	C <sub>4</sub> H <sub>6</sub> Fe <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>8</sub>
0.3437	C <sub>17</sub> H <sub>36</sub> O <sub>2</sub> NI	0.6738	C <sub>6</sub> H <sub>8</sub> O <sub>4</sub>
0.3666	C <sub>17</sub> H <sub>24</sub> O <sub>2</sub>	0.6778	Cu(C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> ) <sub>2</sub> ·2H <sub>2</sub> O
0.3912	C <sub>20</sub> H <sub>30</sub> O <sub>2</sub>	0.6791	C <sub>11</sub> H <sub>23</sub> N·HCl
0.3924	[Br(CH <sub>2</sub> ) <sub>10</sub> C <sub>6</sub> H <sub>5</sub> ] <sub>3</sub> C <sub>3</sub> H <sub>5</sub>	0.6791	[N(C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> ] <sub>2</sub> Pt <sub>2</sub> Br <sub>6</sub>
0.4318	C <sub>8</sub> H <sub>18</sub>	0.6791	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> GeMn(C <sub>6</sub> H <sub>5</sub> ) <sub>5</sub>
0.4371	C <sub>6</sub> H <sub>4</sub> ClC <sub>6</sub> H <sub>5</sub>	0.6826	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> ·2HCl
0.4405	C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>	0.6850	[SFe(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> ] <sub>2</sub>
0.4406	RbH(C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>2</sub>	0.6851	(CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub>
0.4521	C <sub>33</sub> H <sub>62</sub> O <sub>6</sub>	0.6857	C <sub>11</sub> H <sub>17</sub> N·HI
0.4633	C <sub>11</sub> H <sub>23</sub> C <sub>6</sub> H <sub>5</sub>	0.6873	C <sub>10</sub> H <sub>18</sub> (NH <sub>2</sub> ) <sub>2</sub> ·2HCl
0.4647	C <sub>26</sub> H <sub>16</sub>	0.6916	C <sub>8</sub> H <sub>3</sub> BrN <sub>2</sub> ·C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O
0.4701	[(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> As] <sub>2</sub> Re <sub>3</sub> Cl <sub>11</sub>	0.6945	C <sub>2</sub> H <sub>14</sub> N <sub>8</sub> Ni <sub>8</sub> S <sub>2</sub>
0.4746	HI <sub>3</sub> ·2C <sub>6</sub> H <sub>5</sub> C <sub>6</sub> H <sub>5</sub>	0.6975	(N <sub>2</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ·K <sub>2</sub> C <sub>2</sub> H <sub>5</sub>
0.4813	Ca(C <sub>10</sub> H <sub>7</sub> ·HP <sub>6</sub> ) <sub>2</sub> ·3H <sub>2</sub> O	0.6984	C <sub>11</sub> H <sub>23</sub> N·HBr
0.4838	Br·C <sub>6</sub> H <sub>4</sub> ·CH:CH·C <sub>6</sub> H <sub>5</sub>	0.6995	C <sub>14</sub> H <sub>14</sub> Cl <sub>12</sub> Sb <sub>4</sub>
0.4945	C <sub>12</sub> H <sub>4</sub> N <sub>4</sub> ·C <sub>13</sub> H <sub>11</sub> N <sub>2</sub>	0.7016	C <sub>14</sub> H <sub>12</sub> Cl <sub>12</sub> Sb <sub>4</sub>
0.4954	C <sub>22</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> ·0.5CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> C <sub>2</sub> H <sub>5</sub>	0.7027	Se <sub>2</sub> Fe <sub>3</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>6</sub>
0.5044	Fe(H <sub>2</sub> ) <sub>5</sub> (C <sub>2</sub> H <sub>2</sub> NH <sub>3</sub> ) <sub>3</sub> S <sub>6</sub>	0.7028	Na <sub>2</sub> [CuNH <sub>2</sub> (CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ] <sub>2</sub> ·10H <sub>2</sub> O
0.5139	C <sub>10</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>2</sub>	0.7035	CH <sub>3</sub> ·C <sub>6</sub> H <sub>4</sub> ·CH:CH·C <sub>6</sub> H <sub>5</sub>
0.5234	C <sub>6</sub> H <sub>4</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>6</sub> N(CH <sub>3</sub> ) <sub>3</sub> I	0.7091	[C <sub>6</sub> H <sub>5</sub> CH=NH <sub>2</sub> ] <sub>2</sub> SnCl <sub>6</sub>
0.5309	C <sub>22</sub> H <sub>14</sub>	0.7103	C <sub>16</sub> H <sub>6</sub> O <sub>2</sub> Se <sub>2</sub>
0.5430	C <sub>16</sub> H <sub>10</sub> ·C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>6</sub>	0.7106	Te(CSN <sub>2</sub> H <sub>4</sub> ) <sub>4</sub> F <sub>2</sub> ·2H <sub>2</sub> O
0.5442	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> S <sub>2</sub>	0.7109	(NH <sub>4</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub> O <sub>7</sub>
0.5446	NH <sub>2</sub> CS·CSNH <sub>2</sub>	0.7123	Co <sub>3</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>9</sub> C <sub>2</sub> H <sub>3</sub>
0.5463	(Cl·C <sub>6</sub> H <sub>3</sub> CH:CH·N <sub>2</sub> ) <sub>2</sub> Cu	0.7124	C <sub>30</sub> H <sub>42</sub> O <sub>16</sub>
0.5483	Pd[P(C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> ] <sub>2</sub> (CNS) <sub>2</sub>	0.7138	Zn[SC(NHCH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> (NCS) <sub>2</sub>
0.5484	C <sub>6</sub> H <sub>14</sub>	0.7163	(CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub>
0.5490	C <sub>14</sub> H <sub>24</sub>	0.7183	(C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> P <sub>2</sub> S <sub>2</sub>
0.5498	C <sub>14</sub> H <sub>8</sub> Br <sub>2</sub>	0.7188	Zn(SCNH <sub>2</sub> CH <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>
0.5518	Fe <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>6</sub> (C <sub>6</sub> H <sub>5</sub> C=CC <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.7256	Cu(C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> ) <sub>2</sub>
0.5526	C <sub>14</sub> H <sub>8</sub> Br <sub>2</sub>	0.7268	(CH <sub>3</sub> ) <sub>4</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> C <sub>4</sub> Si <sub>2</sub>
0.5627	C <sub>6</sub> H <sub>5</sub> C <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ·Fe <sub>3</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>9</sub>	0.7288	Cl·C <sub>6</sub> H <sub>4</sub> ·CH:CH·C <sub>6</sub> H <sub>5</sub>
0.5688	Re(S <sub>2</sub> C <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ) <sub>3</sub>	0.7312	C <sub>6</sub> H <sub>5</sub> CCC <sub>6</sub> H <sub>5</sub> ·Ge(CH <sub>3</sub> ) <sub>2</sub>
0.5709	Cr(C <sub>6</sub> H <sub>4</sub> N:NC <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> C <sub>5</sub> H <sub>5</sub> NH(C <sub>5</sub> H <sub>5</sub> N) <sub>1/2</sub>	0.7316	C <sub>6</sub> H <sub>10</sub> ·CH <sub>3</sub> HgCl
0.5733	θ <sub>2</sub> IrCl(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> [P(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> ] <sub>2</sub>	0.7322	C <sub>10</sub> H <sub>14</sub> O <sub>5</sub> V
0.5780	Cl·CH=CHHgCl	0.7349	((C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> P) <sub>3</sub> Pt
0.5881	C <sub>10</sub> H <sub>8</sub> ·Fe <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>5</sub>	0.7390	C <sub>6</sub> H <sub>10</sub> ·CH <sub>3</sub> ·HgBr
0.5949	Ru(C <sub>7</sub> H <sub>7</sub> ) <sub>2</sub>	0.7399	Zn(NH <sub>2</sub> CH <sub>2</sub> CO <sub>2</sub> ) <sub>2</sub> ·H <sub>2</sub> O
0.5994	C <sub>4</sub> H <sub>3</sub> N <sub>5</sub> O <sub>2</sub> ·2H <sub>2</sub> O	0.7418	[(C <sub>5</sub> H <sub>4</sub> N·C <sub>5</sub> H <sub>4</sub> N) <sub>2</sub> CuI]I
0.6028	C <sub>15</sub> H <sub>10</sub> N <sub>4</sub> I <sub>4</sub> Na <sub>5</sub> H <sub>2</sub> O	0.7431	C <sub>7</sub> H <sub>9</sub> N <sub>5</sub> :C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>
0.6060	C <sub>6</sub> (N <sub>2</sub> O <sub>2</sub> ) <sub>3</sub> ·C <sub>12</sub> H <sub>12</sub> S <sub>2</sub>	0.7433	Co(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>2</sub>
0.6160	C <sub>14</sub> H <sub>10</sub> Cl <sub>12</sub> S <sub>2</sub>	0.7437	[(CH <sub>3</sub> ) <sub>2</sub> SnCl <sub>2</sub> ] <sub>2</sub> ·C <sub>15</sub> H <sub>11</sub> N <sub>3</sub>
0.6171	Fe <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>6</sub> ·C <sub>12</sub> H <sub>10</sub> N <sub>2</sub>	0.7438	C <sub>18</sub> H <sub>24</sub>
0.6183	(CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> ·2H <sub>2</sub> O	0.7440	C <sub>2</sub> H <sub>2</sub> ·Ge(CH <sub>3</sub> ) <sub>2</sub>



$\bar{P}1$   $C_1^1$  No. 2 (continued)

## Organic (continued)

0.7443	$((C_6H_5)_2PH)_3NiBr_2$	0.8451	$C_6H_9N_3 \cdot 2HCl \cdot H_2O$
0.7443	$((C_6H_5)_2PH)_3CoBr_2$	0.8459	$C_6H_{10}O \cdot CH_3 \cdot HgBr$
0.7454	$Cu(CH_3CH_2CH_2COO)_2$	0.8464	$C_6H_5N_5O$
0.7476	$C_6H_{10}O \cdot C_6H_{10}$	0.8476	$C_6H_7N_5 \cdot C_5H_5BrN_2O_2$
0.7491	$C_{10}H_{12}O_6$	0.8482	$C_6H_{10}O \cdot CH_3 \cdot HgCl$
0.7498	$Ni(NCS)_2(NH_2CSNH_2)_2$	0.8484	$C_{30}H_{18}Cl_2$
0.7504	$Co_2(CO)_9C_2H_2$	0.8489	$(C_3H_6N_2S)_4CuNO_3$
0.7507	$C_6H_{10}O \cdot CH_3 \cdot HgI$	0.8494	$C_6H_{10}O \cdot CH_3 \cdot HgI$
0.7518	$C_6H_4-COOH-N=N-C_6H_4N(CH_3)_2$	0.8504	$(C_6H_5)_6P_6$
0.7578	$C_{14}Cl_5H_9$	0.8505	$C_{12}H_{10}(Cr(CO)_3)_2$
0.7589	$Cu(HCOO)_2 \cdot 0.5(C_4H_8O_2)$	0.8509	$Sb(C_6H_5)_3$
0.7615	$C_{13}H_{14}NO_2Br$	0.8532	$NH_2NHCNH_2$
0.7617	$Cd(N_2H_4)_2(CH_3COO)_2$	0.8536	$C_8H_{10}O_4$
0.7623	$C_{12}H_{20}N_4O_8P_2S_3O_2H_2O$	0.8562	$C_2H_5O \cdot C_6H_4 \cdot CH:CH \cdot COOH$
0.7637	$((C_6H_5)_2PH)_3NiI_2$	0.8564	$Cu(CH_3CH_2COO)_2$
0.7637	$((C_6H_5)_2PH)_3CoI_2$	0.8574	$(C_5H_6O_2)_2Cr[OP(C_6H_5)_2O]_2Cr(C_5H_6O_2)_2$
0.7646	$C_7H_9N_5 \cdot C_5H_5BrN_2O_2$	0.8590	$[(C_6H_5)_3CSFe(CO)_3]_2$
0.7659	$CH_3COOCl$	0.8590	$CH_3 \cdot Br \cdot C_4H_2N_2O_2 \cdot CH_3 \cdot C_5H_2N_4 \cdot NH_2$
0.7668	$(C_4H_9)_2C_4H_2OBr_2$	0.8600	$As(C_6H_5)_3$
0.7678	$Al_2Br_6 \cdot C_6H_6$	0.8605	$C_{12}H_{24}Cl_2N_8S_4Te$
0.7709	$Mn(N_2H_4)_2(CH_3COO)_2$	0.8634	$(CH_3)_2C_6H_6Cl_2$
0.7716	$(C_6H_5)_5Sb$	0.8652	$C_8F_{12}$
0.7723	$Zn(N_2H_4)_2(CH_3COO)_2$	0.8657	$KC_6H_5O_6$
0.7728	$Ni(C_2H_7N_5)_2Cl_2 \cdot 2H_2O$	0.8662	$Te(C_5H_{12}N_2S)_2Br_2$
0.7742	$CH_2F \cdot CO \cdot NH_2$	0.8668	$HOO \cdot C \cdot CH(CH_3) \cdot CH(CH_3) \cdot COOH$
0.7755	$C_{14}H_{10} \cdot C_{10}H_2O_6$	0.8671	$KH_2C_6H_5O_7$
0.7794	$C_6(CH_3)_6$	0.8682	$[(C_6H_5)_2SiO]_4$
0.7859	$C_4H_2N_3O_4Rb$	0.8682	$Te(C_5H_{12}N_2S)_2Cl_2$
0.7868	$(CH_3)_2AsCN$	0.8690	$C_36H_36N_4NiO_6 \cdot 0.5C_6H_6$
0.7911	$SeOCl_2 \cdot 2C_5H_5N$	0.8710	$Cu(C_6H_9O)_2$
0.7912	$C_{21}H_{35}N_3$	0.8720	$C_5H_9I_3N_3$
0.7912	$C_{23}H_{22}O_6$	0.8721	$[(C_4H_9)_4N]_2Co(C_4N_2S_2)_2$
0.7958	$C_7H_9N_5O \cdot C_5H_7N_3O$	0.8763	$C_6H_4Cl_2$
0.7983	$Ni(NH_2CH_2CH_2COO)_2 \cdot 2H_2O$	0.8770	$C_4H_6O_6 \cdot C_4H_6O_6 \cdot 2H_2O$
0.8013	$C_4(CH)_2(COOH)_2(COOCC_2H_5)_6$	0.8793	$C_4H_6O_6 \cdot C_4H_6O_6 \cdot 2H_2O$
0.8038	$BrC_6H_3(CH_3)NHSO_2C_6H_5$	0.8803	$C_{15}H_{10}NO_3Br$
0.8059	$C_4H_{10}N_2 \cdot 2(HCl \cdot ICl)$	0.8810	$(C_5H_6N)_2(AsF_4O)_2$
0.8062	$C_{40}H_{30}BrN_3O_3$	0.8825	$(C_6H_5)_3PAuCo(CO)_4$
0.8097	$ClCH_2NC_5H_4CH=NOH$	0.8847	$Cu(C_8H_{14}N_6S_2)$
0.8097	$BrCH_2NC_5H_4CH=NOH$	0.8848	$NH_2CONHNHCOOH$
0.8112	$C_5H_4NOCH_2OH \cdot HCl$	0.8900	$HOOCCCH_2CH(CH_3)CH(CH_3)CH_2COOH$
0.8113	$HgCl_2 \cdot C_4H_8$	0.8908	$Ti(OCH_3)_4$
0.8121	$(CH_3)_2C:N \cdot NH \cdot C_6H_3(NO_2)_2$	0.8921	$[(NO_2)_2C_6O_4](NH_4)_2$
0.8125	$[CH(OH)COOH]_2 \cdot H_2O$	0.8921	$RuCl_2C_{10}H_{16}$
0.8137	$C_{28}H_{18}O_4$	0.8923	$KNaC_4H_4O_6 \cdot 4H_2O$
0.8137	$Rb_2C_2H_2O_4 \cdot H_2O$	0.8925	$Cu(CH_3CH_2COO)_2$
0.8154	$C_{34}H_{32}ClFeN_4O_4$	0.8927	$Se[(C_2H_5O)_2PS_2]_2$
0.8157	$C_{34}H_{32}BrFeN_4O_4$	0.8929	$BrC_6H_4 \cdot C_2HN_2O_2$
0.8159	$(C_5H_5)_2Mo_2H[P(CH_3)_2](CO)_4$	0.8936	$C_{11}H_{11}CuNO_2$
0.8178	$C_9H_7NOHCl \cdot H_2O$	0.8941	$C_8H_{10}N_2O_2$
0.8183	$Ba_2Cu(HCOO)_6 \cdot 4H_2O$	0.8947	$(OC_6H_4CH=NCH_3)_2Mn$
0.8196	$Pt(C_2H_8N_2)_2Cl_2$	0.8961	$C_{40}H_{52}O_2$
0.8205	$Cu_2(NH_2CH_3)_4(OH)_2SO_4 \cdot H_2O$	0.8966	$C_4H_8N_2O_2$
0.8206	$PdCl_2 \cdot 2C_2H_8N_2$	0.8982	$Mo(CH_3COO)_2$
0.8211	$Cu(C_{13}H_{11}N_4S)_2$	0.9017	$C_{25}H_{30}N_5NiCl \cdot xH_2O \cdot yCH_3OH$
0.8228	$C_{12}H_8O_4S_2$	0.9027	$C_{23}H_{27}N_2O_2S_2Br$
0.8239	$C_4H_6Cl_2O_2$	0.9030	$C_{14}H_{12}O$
0.8246	$(CH_3OHCCH_2)_2$	0.9038	$(OC_6H_4CH=NCH_3)_2Co$
0.8252	$[Pt(C_2H_8N_2)_2]Cl_2$	0.9041	$HN(C_2H_5)_3 \cdot HF \cdot e_3(CO)_{11}$
0.8288	$C_6H_6O_4$	0.9056	$Cu(C_8H_2ClCOO)_2 \cdot 2C_9H_7N$
0.8301	$C_4H_4N_2O_5$	0.9057	$Te(C_5H_{12}N_2S)Br_2$
0.8344	$[Zn_9(OH)_{22}]Zn_4(OH, H_2O)_8[C_6H_3(NO_2)_2O]_4$	0.9070	$Pb \cdot S_2O_3 \cdot SSC(NHCH_2)_2$
0.8357	$C_{11}H_{23}COOH$	0.9092	$C_{10}H_{10}$
0.8364	$(C_{14}H_8BrO)_2$	0.9098	$CdCl_2 \cdot 2HCOONH_2$
0.8367	$Cu_2Cl_2 \cdot (C_8H_{12})_2$	0.9098	$Te(C_5H_{12}N_2S)Cl_2$
0.8370	$C_8HBrN_4O_5S$	0.9110	$CH_3O \cdot C_6H_4 \cdot CH:CH \cdot COOH$
0.8397	$C_{30}H_{18}Br_2O_7$	0.9122	$C_{24}H_{15}N_4O_5P \cdot C_6H_6$
0.8413	$(C_8H_{12})_2Ni$	0.9125	$PCH_3(C_6H_5)_3Ni[S_2C_2(CN)_2]_2$
0.8419	$C_4H_8O_2 \cdot C_2I_2$	0.9128	$(ClC_6H_4)_2TeI_2$
0.8431	$C_{44}H_{30}N_4$	0.9130	$C_{23}H_{28}IN_3O$
0.8436	$C_{44}H_{28}AgN_4$	0.9138	$CaC_{10}H_{12}N_2O_6 \cdot xH_2O$
0.8442	$CH_3 \cdot C_6H_4 \cdot CH:CH \cdot COOH$	0.9157	$C_6H_4Cl_3I$
0.8442	$(C_6H_6NO)_2Pd \cdot C_6Cl_4O_2$	0.9159	$Zn(C_8H_8NO)_2$
0.8446	$C_{14}H_{10}(C_2Cl_4)_2$	0.9162	$(C_6H_5)_3P \cdot O \cdot C_6H_2N_6O_4$

P1 C<sub>1</sub><sup>1</sup> No. 2 (continued)

## Organic (continued)

0.9210	(C <sub>6</sub> NH <sub>2</sub> ) <sub>2</sub>	0.9701	(C <sub>6</sub> H <sub>5</sub> CN) <sub>2</sub> PdCl <sub>2</sub>
0.9221	HgCl <sub>2</sub> •2CH <sub>3</sub> OH	0.9703	C <sub>14</sub> H <sub>12</sub> Cl <sub>6</sub> Cl <sub>2</sub> S
0.9228	(C <sub>6</sub> NH <sub>2</sub> ) <sub>2</sub>	0.9706	[(CH <sub>3</sub> ) <sub>4</sub> N] <sub>2</sub> •Ni(C <sub>4</sub> H <sub>2</sub> N <sub>2</sub> S <sub>2</sub> ) <sub>2</sub>
0.9228	C <sub>2</sub> H <sub>2</sub> •Ge(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.9709	K <sub>2</sub> Cu(C <sub>2</sub> Cl <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> O
0.9298	C <sub>3</sub> H <sub>5</sub> •C <sub>6</sub> H <sub>4</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>	0.9713	C <sub>10</sub> H <sub>5</sub> Cl <sub>3</sub>
0.9299	Cu(C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> ) <sub>2</sub> (SCN) <sub>2</sub>	0.9729	C <sub>5</sub> H <sub>7</sub> N <sub>3</sub> Cl
0.9307	Pd(C <sub>6</sub> H <sub>6</sub> N <sub>6</sub> ) <sub>2</sub> •C <sub>6</sub> H <sub>2</sub> (CN) <sub>4</sub>	0.9730	BrC <sub>6</sub> H <sub>4</sub> N <sub>2</sub>
0.9319	C <sub>12</sub> H <sub>8</sub> BrCl	0.9731	NaHC <sub>2</sub> Cl <sub>4</sub> •H <sub>2</sub> O
0.9334	[(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> As][ReBr <sub>4</sub> (CH <sub>3</sub> CN)]	0.9731	C <sub>10</sub> H <sub>5</sub> Br(CH <sub>3</sub> ) <sub>2</sub>
0.9349	C <sub>16</sub> H <sub>18</sub> N <sub>3</sub> SI•3H <sub>2</sub> O	0.9735	Ca[(C <sub>7</sub> H <sub>5</sub> Cl <sub>3</sub> N) <sub>2</sub> Al(OH)(OH <sub>2</sub> )]•7H <sub>2</sub> O
0.9353	C <sub>17</sub> H <sub>23</sub> Br <sub>4</sub> S	0.9740	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>
0.9354	C <sub>14</sub> H <sub>14</sub> Cl <sub>4</sub> S <sub>2</sub>	0.9766	P(C <sub>9</sub> H <sub>9</sub> NS) <sub>2</sub> Cl <sub>4</sub>
0.9355	2HgCl <sub>2</sub> •(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> S	0.9770	Cu <sub>2</sub> Cl <sub>2</sub> •C <sub>2</sub> H <sub>6</sub> N <sub>2</sub>
0.9361	C <sub>9</sub> H <sub>8</sub> O <sub>5</sub>	0.9773	[(CF <sub>3</sub> ) <sub>2</sub> C <sub>2</sub> S <sub>2</sub> CoS <sub>2</sub> C <sub>2</sub> (CF <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub>
0.9394	(C <sub>6</sub> H <sub>11</sub> ) <sub>2</sub> PS•PS(C <sub>6</sub> H <sub>11</sub> ) <sub>2</sub>	0.9782	[(C <sub>6</sub> H <sub>11</sub> ) <sub>3</sub> P] <sub>2</sub> NiCl <sub>2</sub>
0.9403	(C <sub>8</sub> H <sub>13</sub> )Ni(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> )	0.9785	Br•C <sub>6</sub> H <sub>3</sub> •(C <sub>6</sub> H <sub>5</sub> )•C <sub>8</sub> H <sub>4</sub> N <sub>2</sub> •H <sub>2</sub> O
0.9405	(CH <sub>2</sub> •C <sub>6</sub> NH) <sub>6</sub> •0.5H <sub>2</sub> O	0.9791	Te(C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> S) <sub>4</sub> (Cl <sub>4</sub> ) <sub>2</sub>
0.9409	C <sub>6</sub> H <sub>4</sub> •CH=CH•C <sub>6</sub> H <sub>5</sub>	0.9796	IC <sub>6</sub> H <sub>3</sub> (C <sub>6</sub> H <sub>5</sub> )•C <sub>8</sub> H <sub>4</sub> N <sub>2</sub> •H <sub>2</sub> O
0.9409	C <sub>8</sub> H <sub>6</sub> N <sub>4</sub> Cl <sub>2</sub> •2H <sub>2</sub> O	0.9796	MoCl <sub>2</sub> (C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>2</sub>
0.9431	C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	0.9797	C <sub>23</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>
0.9433	Cu(OCCH <sub>2</sub> CH <sub>2</sub> CO) <sub>2</sub> •2H <sub>2</sub> O	0.9827	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> (OH) <sub>2</sub> CuCl <sub>2</sub>
0.9444	Br(CH <sub>2</sub> ) <sub>10</sub> CO <sub>2</sub> H	0.9830	Pt(C <sub>2</sub> H <sub>7</sub> N <sub>5</sub> ) <sub>3</sub> (Cl <sub>4</sub> ) <sub>2</sub>
0.9451	C <sub>12</sub> Cl <sub>12</sub>	0.9833	Ni(SC <sub>2</sub> H <sub>4</sub> OH) <sub>2</sub>
0.9452	(CH <sub>3</sub> ) <sub>3</sub> (C <sub>7</sub> H <sub>5</sub> O <sub>2</sub> )Pt	0.9834	(NH <sub>4</sub> ) <sub>2</sub> Cu(C <sub>2</sub> Cl <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> O
0.9456	K <sub>3</sub> ReCl <sub>2</sub> (CN) <sub>4</sub>	0.9841	C <sub>2</sub> N <sub>2</sub> Si(C <sub>6</sub> NH <sub>2</sub> ) <sub>2</sub>
0.9458	Cu <sub>2</sub> S <sub>2</sub> O <sub>3</sub> •6SC(NH <sub>2</sub> )CH <sub>3</sub>	0.9854	(PdAl <sub>2</sub> Cl <sub>7</sub> C <sub>6</sub> H <sub>6</sub> ) <sub>2</sub>
0.9465	C <sub>18</sub> H <sub>26</sub> FeN <sub>6</sub> Cl <sub>4</sub> •2H <sub>2</sub> O	0.9860	CaS <sub>4</sub> •4C <sub>6</sub> (NH <sub>2</sub> ) <sub>2</sub>
0.9471	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> Ge(CH) <sub>4</sub> Ge(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.9865	C <sub>18</sub> H <sub>37</sub> CO <sub>2</sub> H
0.9488	C <sub>4</sub> H <sub>6</sub> Cl <sub>4</sub>	0.9879	(CH <sub>3</sub> ) <sub>2</sub> As <sub>2</sub> OH
0.9488	Cr(C <sub>6</sub> ) <sub>3</sub> •C <sub>18</sub> H <sub>16</sub> O <sub>2</sub>	0.9885	C <sub>21</sub> H <sub>21</sub> ClN <sub>2</sub> S <sub>2</sub>
0.9501	N <sub>2</sub> O <sub>4</sub> •C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	0.9893	CH <sub>3</sub> CO•C <sub>6</sub> H <sub>4</sub> •CH(C <sub>2</sub> H <sub>5</sub> )•CH(C <sub>2</sub> H <sub>5</sub> )C <sub>6</sub> H <sub>4</sub> COCH <sub>3</sub>
0.9524	Fe(C <sub>5</sub> H <sub>5</sub> N) <sub>6</sub> •Fe <sub>4</sub> (C <sub>6</sub> ) <sub>13</sub>	0.9897	Mn[SC(NHCH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> (NCS) <sub>2</sub>
0.9524	C <sub>7</sub> H <sub>12</sub> Cl <sub>4</sub>	0.9909	C <sub>14</sub> H <sub>8</sub> Cl <sub>4</sub> N <sub>2</sub>
0.9526	PtI[(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> AsC <sub>6</sub> H <sub>4</sub> ] <sub>3</sub> As[(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> ]	0.9916	C <sub>30</sub> H <sub>44</sub> Cl <sub>16</sub>
0.9528	C <sub>17</sub> H <sub>12</sub> S <sub>3</sub>	0.9935	UO <sub>2</sub> (NO <sub>3</sub> ) <sub>2</sub> [(C <sub>2</sub> H <sub>5</sub> O) <sub>3</sub> PO] <sub>2</sub>
0.9537	H <sub>2</sub> OCCH:CHCO <sub>2</sub> H	0.9938	Br <sub>2</sub> C <sub>6</sub> H <sub>3</sub> •C(CN):CH•C <sub>6</sub> H <sub>5</sub>
0.9556	C <sub>40</sub> H <sub>50</sub> O <sub>2</sub>	0.9949	CaBr <sub>2</sub> •2[(CH <sub>2</sub> ) <sub>6</sub> N <sub>4</sub> ] <sub>2</sub> •10H <sub>2</sub> O
0.9606	H <sub>2</sub> C:N•NH•C <sub>6</sub> H <sub>3</sub> (NO <sub>2</sub> ) <sub>2</sub>	0.9955	C <sub>16</sub> Cl <sub>3</sub> H <sub>15</sub> O <sub>2</sub>
0.9614	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> •C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	0.9958	C <sub>8</sub> H <sub>11</sub> N <sub>3</sub> •HCl
0.9618	(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>2</sub> O <sub>2</sub>	0.9970	C <sub>8</sub> H <sub>11</sub> Pd(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> )
0.9620	Ag <sub>3</sub> (NO <sub>3</sub> ) <sub>2</sub> SCN	0.9974	[C <sub>18</sub> H <sub>12</sub> N <sub>2</sub> PdS <sub>2</sub> ]
0.9636	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	0.9975	Ni(NCS) <sub>2</sub> •2C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> S
0.9661	HgCl <sub>2</sub> •C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	0.9976	(C <sub>6</sub> )Ni•C <sub>5</sub> H <sub>10</sub> N-CN
0.9677	(C <sub>21</sub> H <sub>19</sub> As <sub>2</sub> )Br•C <sub>2</sub> H <sub>8</sub> O <sub>2</sub>	0.9986	CaC <sub>2</sub>
0.9685	KC(CN) <sub>3</sub>	0.9986	(NH <sub>2</sub> ) <sub>3</sub> C <sub>6</sub> (NO <sub>2</sub> ) <sub>3</sub>
0.9687	Na <sub>4</sub> Ni(NCS) <sub>6</sub> •12H <sub>2</sub> O	1.0000	MgCl <sub>2</sub> •2(CH <sub>2</sub> ) <sub>6</sub> N <sub>4</sub> •10H <sub>2</sub> O
		1.0000	[(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> PCH <sub>3</sub> ] <sub>3</sub> Pt(SnCl <sub>3</sub> ) <sub>5</sub>

2

P2 C<sub>2</sub><sup>1</sup> No. 3Inorganic - 4  
Organic - 11

## Inorganic

1.0838	Ca <sub>0.5</sub> Na <sub>0.5</sub> Mg <sub>0.5</sub> Al <sub>0.5</sub> Si <sub>2</sub> O <sub>6</sub>	5.3286	Nb <sub>2</sub> O <sub>5</sub>
1.5064	PbMnOH <sub>2</sub>	6.0152	Nb <sub>17</sub> Cl <sub>42</sub> F

## Organic

0.3934	C <sub>18</sub> H <sub>17</sub> Cl <sub>6</sub> •0.5CHCl <sub>3</sub>	2.5509	C <sub>17</sub> H <sub>22</sub> N <sub>2</sub> O <sub>6</sub> S•H <sub>2</sub> O
0.9957	C <sub>11</sub> H <sub>14</sub> Cl <sub>6</sub> N <sub>2</sub>	2.6072	C <sub>18</sub> H <sub>24</sub> N <sub>2</sub>
1.3409	C <sub>6</sub> H <sub>8</sub> Cl <sub>6</sub> (CH <sub>3</sub> CO) <sub>4</sub>	3.4249	C <sub>5</sub> H <sub>11</sub> N <sub>2</sub> O <sub>2</sub> S
2.0251	[C <sub>15</sub> H <sub>25</sub> O <sub>2</sub> Br <sub>2</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> ]	3.5038	C <sub>12</sub> H <sub>16</sub> N <sub>4</sub> O <sub>9</sub> •C <sub>5</sub> H <sub>5</sub> N
2.2073	C <sub>10</sub> H <sub>13</sub> BrN <sub>2</sub> Cl <sub>4</sub>	5.7491	C <sub>7</sub> H <sub>11</sub> Cl <sub>3</sub> O <sub>3</sub>
2.4690	C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> Cl <sub>4</sub> S <sub>2</sub> •0.5H <sub>2</sub> O		

2

P2<sub>1</sub> C<sub>2</sub><sup>2</sup> No. 4Inorganic - 42  
Organic - 458

## Inorganic

0.1189	Pb <sub>9</sub> As <sub>13</sub> S <sub>28</sub>	0.3267	Pb <sub>7</sub> As <sub>9</sub> S <sub>20</sub>
0.1360	(Ca,Sr)B <sub>6</sub> O <sub>10</sub> •3H <sub>2</sub> O	0.5003	KD <sub>2</sub> PO <sub>4</sub>
0.3252	Pb <sub>2</sub> As <sub>2</sub> S <sub>5</sub>	0.5074	Ag <sub>2</sub> CO <sub>3</sub>

P<sub>2</sub><sub>1</sub> C<sub>2</sub><sup>2</sup> No. 4 (continued)

## Inorganic (continued)

0.6140	P <sub>4</sub> S <sub>5</sub>	1.4523	C <sub>18</sub> H <sub>32</sub>
0.6167	Ba <sub>2</sub> Al <sub>4</sub> Si <sub>12</sub> O <sub>32</sub> •12H <sub>2</sub> O	1.5605	AgTmS <sub>2</sub>
0.6258	W <sub>2</sub> O <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>	1.5613	BaCa(CO <sub>3</sub> ) <sub>2</sub>
0.6279	AlCl <sub>6</sub>	1.5623	AgErS <sub>2</sub>
0.6912	BiPO <sub>4</sub>	1.5673	AgHoS <sub>2</sub>
0.7216	UO <sub>3</sub>	1.5690	AgDyS <sub>2</sub>
0.7612	S <sub>3</sub> N <sub>2</sub> Cl <sub>2</sub>	1.5692	AgYs <sub>2</sub>
0.8790	Pd(NH <sub>3</sub> ) <sub>2</sub> (NO <sub>2</sub> ) <sub>2</sub>	1.5718	AgGdS <sub>2</sub>
0.9663	NH <sub>4</sub> HN <sub>2</sub> O <sub>2</sub>	1.5740	AgTbS <sub>2</sub>
1.1065	PPd <sub>4.8</sub>	1.5835	AgSmS <sub>2</sub>
1.1305	NaBSi <sub>2</sub> O <sub>6</sub> •H <sub>2</sub> O	1.6827	Li <sub>2</sub> SO <sub>4</sub> •H <sub>2</sub> O
1.1959	Mg <sub>2</sub> (Sr, Ca) <sub>4</sub> B <sub>24</sub> O <sub>42</sub> •9H <sub>2</sub> O	1.6853	Li <sub>2</sub> SO <sub>4</sub> •H <sub>2</sub> O
1.3575	CaK <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •H <sub>2</sub> O	1.9178	Na <sub>2</sub> SiO <sub>3</sub> •6H <sub>2</sub> O
1.3842	Sr <sub>3</sub> UO <sub>6</sub>	2.1983	NaPO <sub>3</sub>
1.3931	Ca <sub>3</sub> UO <sub>6</sub>	2.2500	Ca(H <sub>3</sub> O) <sub>2</sub> (UO <sub>2</sub> SiO <sub>4</sub> ) <sub>2</sub> •3H <sub>2</sub> O
1.4014	(Al, Mg, Fe, Ca) <sub>4</sub> Si <sub>2</sub> O <sub>9</sub> (OH)	2.7719	NH <sub>4</sub> H <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub>
1.4140	Ca <sub>4</sub> Al <sub>2</sub> (OH) <sub>14</sub> •6H <sub>2</sub> O	3.0999	Pb <sub>6</sub> As <sub>10</sub> S <sub>20</sub>
1.4447	C <sub>19</sub> H <sub>34</sub>	3.2575	Ca <sub>2</sub> Na(Ti, Ce)F(SiO <sub>4</sub> ) <sub>2</sub>

## Organic

0.1465	C <sub>21</sub> H <sub>32</sub> O <sub>3</sub>	0.6934	C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>
0.1683	C <sub>19</sub> H <sub>30</sub> O	0.7020	C <sub>32</sub> H <sub>52</sub> O <sub>2</sub>
0.1761	C <sub>21</sub> H <sub>28</sub> O <sub>2</sub>	0.7039	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub> •H <sub>2</sub> O
0.2375	C <sub>14</sub> H <sub>20</sub> O <sub>7</sub> S	0.7090	(CO) <sub>3</sub> C <sub>8</sub> H <sub>10</sub> Cr
0.2425	C <sub>27</sub> H <sub>46</sub> N <sub>2</sub> O	0.7094	(CH <sub>3</sub> ) <sub>4</sub> C <sub>6</sub> H <sub>6</sub> O <sub>6</sub>
0.2446	(CH <sub>3</sub> ) <sub>2</sub> (CH) <sub>2</sub> (NH <sub>2</sub> )COOH	0.7169	(CH <sub>2</sub> •NH <sub>2</sub> •COOH) <sub>3</sub> H <sub>2</sub> BeF <sub>4</sub>
0.2987	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>	0.7221	(CH <sub>2</sub> •NH <sub>2</sub> •COOH) <sub>3</sub> H <sub>2</sub> SeO <sub>4</sub>
0.2995	HC <sub>19</sub> H <sub>29</sub> O	0.7265	(C <sub>4</sub> H <sub>8</sub> )(C <sub>6</sub> H <sub>5</sub> CHCH <sub>3</sub> NH <sub>2</sub> )PtCl <sub>2</sub>
0.3039	C <sub>19</sub> H <sub>30</sub> O <sub>2</sub>	0.7497	C <sub>6</sub> H <sub>6</sub> (OH) <sub>6</sub>
0.3217	C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub> HCl•H <sub>2</sub> O	0.7551	C <sub>11</sub> H <sub>11</sub> N <sub>2</sub> O <sub>3</sub>
0.3326	C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> •HBr•0.5H <sub>2</sub> O	0.7629	C <sub>11</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>
0.3592	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub> •H <sub>2</sub> O	0.7868	C <sub>64</sub> H <sub>90</sub> N <sub>12</sub> O <sub>16</sub>
0.3706	C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> •HCl	0.7900	Mo <sub>2</sub> O <sub>3</sub> (S <sub>2</sub> C <sub>6</sub> C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub>
0.3834	C <sub>20</sub> H <sub>24</sub> O <sub>2</sub> N <sub>2</sub> •C <sub>6</sub> H <sub>6</sub>	0.7934	C <sub>21</sub> H <sub>25</sub> BrO <sub>3</sub>
0.3918	C <sub>18</sub> H <sub>24</sub> O <sub>2</sub>	0.7950	(ClC <sub>6</sub> H <sub>4</sub> )CH <sub>2</sub> C(CN) <sub>2</sub>
0.3974	CSe(NH•NH <sub>2</sub> ) <sub>2</sub>	0.8007	C <sub>6</sub> H <sub>7</sub> (OH) <sub>5</sub>
0.3974	C <sub>18</sub> H <sub>21</sub> (OH) <sub>3</sub>	0.8070	C <sub>45</sub> H <sub>51</sub> IN <sub>2</sub> O <sub>14</sub> •C <sub>2</sub> H <sub>6</sub> OS•H <sub>2</sub> O
0.3987	C <sub>18</sub> H <sub>22</sub> O <sub>2</sub>	0.8248	C <sub>15</sub> H <sub>25</sub> BrN <sub>2</sub>
0.4024	Br(NO <sub>2</sub> )C <sub>6</sub> H <sub>3</sub> COCH <sub>2</sub> C•CH	0.8249	CH <sub>3</sub> CH <sub>2</sub> COCH(NH <sub>2</sub> )CH <sub>2</sub> SH•HCl•CO(NH <sub>2</sub> ) <sub>2</sub>
0.4086	C <sub>17</sub> H <sub>21</sub> BrO <sub>5</sub>	0.8252	C <sub>33</sub> H <sub>38</sub> N <sub>4</sub> O <sub>2</sub>
0.4172	HOC <sub>18</sub> H <sub>21</sub> O	0.8366	C <sub>6</sub> H <sub>13</sub> N <sub>5</sub> O•HCl
0.4523	C <sub>21</sub> H <sub>32</sub> O <sub>5</sub>	0.8396	C <sub>15</sub> H <sub>26</sub> N <sub>2</sub> O•HBr
0.4542	C <sub>34</sub> H <sub>16</sub> O <sub>2</sub>	0.8425	C <sub>21</sub> H <sub>13</sub> N
0.4584	C <sub>11</sub> H <sub>17</sub> N <sub>3</sub> O <sub>8</sub>	0.8442	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>
0.4737	C <sub>19</sub> H <sub>26</sub> O <sub>2</sub>	0.8442	C <sub>18</sub> H <sub>21</sub> N <sub>2</sub> O <sub>2</sub>
0.5043	C <sub>47</sub> H <sub>59</sub> IN <sub>4</sub> O <sub>10</sub> •2H <sub>2</sub> O	0.8538	C <sub>20</sub> H <sub>31</sub> ON•CH <sub>3</sub> I
0.5074	As <sub>2</sub> CO <sub>3</sub>	0.8584	NH <sub>2</sub> •CH <sub>2</sub> •COOH
0.5121	[(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> O] <sub>3</sub> I	0.8693	C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> O <sub>2</sub> •H <sub>2</sub> O
0.5282	C <sub>6</sub> H <sub>5</sub> CH(CH <sub>3</sub> )NH <sub>2</sub> •C <sub>4</sub> H <sub>6</sub> O <sub>6</sub>	0.8857	C <sub>19</sub> H <sub>30</sub> OH•CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>
0.5605	C <sub>24</sub> H <sub>24</sub> O <sub>12</sub> •HBr	0.8902	C <sub>9</sub> H <sub>16</sub> O <sub>6</sub>
0.5607	C <sub>24</sub> H <sub>24</sub> O <sub>12</sub> •HI	0.8987	C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
0.5625	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> •HCl•2H <sub>2</sub> O	0.8994	C <sub>20</sub> H <sub>27</sub> N <sub>3</sub> •HBr
0.5672	C <sub>15</sub> H <sub>25</sub> Cl	0.9080	C <sub>6</sub> H <sub>8</sub> O <sub>6</sub>
0.5692	N(CH <sub>3</sub> ) <sub>4</sub> HgBr <sub>3</sub>	0.9097	C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub> Br <sub>2</sub>
0.5764	C <sub>15</sub> H <sub>25</sub> Br	0.9137	C <sub>22</sub> H <sub>33</sub> N <sub>5</sub> •HBr
0.5816	C <sub>15</sub> H <sub>26</sub> N <sub>2</sub> •F <sub>2</sub> SO <sub>4</sub> •5H <sub>2</sub> O	0.9192	C <sub>28</sub> H <sub>39</sub> N <sub>5</sub> O <sub>8</sub>
0.5845	C <sub>15</sub> H <sub>24</sub> O <sub>2</sub>	0.9214	(CH <sub>3</sub> ) <sub>2</sub> N•C <sub>6</sub> H <sub>4</sub> •NO <sub>2</sub>
0.5960	C <sub>6</sub> H <sub>5</sub> OH	0.9249	C <sub>18</sub> H <sub>26</sub> BrNO <sub>6</sub> •0.5C <sub>2</sub> H <sub>5</sub> OH
0.5984	C <sub>5</sub> H <sub>9</sub> N <sub>3</sub> •2HCl	0.9273	C <sub>2</sub> H <sub>5</sub> CHNH <sub>3</sub> CH <sub>2</sub> SSO <sub>3</sub>
0.5988	C <sub>25</sub> H <sub>39</sub> NO <sub>6</sub> •HI	0.9285	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>
0.6109	C <sub>19</sub> H <sub>24</sub> N <sub>7</sub> O <sub>12</sub> P•4H <sub>2</sub> O	0.9315	C <sub>22</sub> H <sub>33</sub> N <sub>5</sub> O
0.6162	C <sub>22</sub> H <sub>33</sub> N <sub>5</sub> •HBr•H <sub>2</sub> O	0.9460	C <sub>6</sub> H <sub>8</sub> Br <sub>4</sub>
0.6322	C <sub>13</sub> H <sub>22</sub> O <sub>7</sub>	0.9463	C <sub>5</sub> H <sub>9</sub> N <sub>3</sub>
0.6464	[Au(C <sub>5</sub> H <sub>5</sub> N) <sub>2</sub> Cl <sub>2</sub> ]Cl•H <sub>2</sub> O	0.9494	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>6</sub>
0.6492	(C <sub>6</sub> H <sub>5</sub> PS) <sub>3</sub>	0.9506	CH <sub>2</sub> OH(CHOH) <sub>4</sub> COONa
0.6562	Na <sub>2</sub> PO <sub>4</sub> C <sub>3</sub> H <sub>5</sub> (OH) <sub>2</sub> •5H <sub>2</sub> O	0.9618	C <sub>27</sub> H <sub>42</sub> O <sub>8</sub>
0.6687	C <sub>26</sub> H <sub>34</sub> O <sub>3</sub>	0.9811	C <sub>15</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub>
0.6787	C <sub>19</sub> H <sub>29</sub> •CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>	0.9867	C <sub>5</sub> H <sub>9</sub> O <sub>5</sub> SNCu•4H <sub>2</sub> O
0.6806	C <sub>19</sub> H <sub>12</sub> O <sub>2</sub>	0.9889	C <sub>5</sub> H <sub>11</sub> SO <sub>5</sub> N
0.6821	CuCl <sub>2</sub> •2C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> •2H <sub>2</sub> O	0.9899	C <sub>19</sub> H <sub>26</sub> NO <sub>2</sub> •HCl
0.6826	C <sub>6</sub> H <sub>11</sub> NO <sub>3</sub> SO <sub>2</sub> •HCl•H <sub>2</sub> O	0.9961	C <sub>6</sub> H <sub>5</sub> •CH <sub>2</sub> •(C <sub>3</sub> H <sub>2</sub> N <sub>2</sub> )CHCOH(CH <sub>3</sub> ) <sub>2</sub> SH•HCl
0.6853	C <sub>25</sub> H <sub>37</sub> NO <sub>6</sub>	0.9995	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub> •H <sub>2</sub> O
0.6884	C <sub>15</sub> H <sub>16</sub> BrO <sub>3</sub>	1.0060	C <sub>5</sub> H <sub>5</sub> •Co•C <sub>5</sub> H <sub>4</sub> CO <sub>2</sub> C <sub>6</sub> H <sub>5</sub>

## Organic (continued)

1.0081	C <sub>41</sub> H <sub>48</sub> N <sub>4</sub> O <sub>4</sub> •CH <sub>3</sub> OH	1.3017	C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> •HBr•H <sub>2</sub> O
1.0158	C <sub>21</sub> H <sub>32</sub> O <sub>2</sub>	1.3092	C <sub>2</sub> H <sub>5</sub> NH <sub>3</sub> I
1.0194	C <sub>8</sub> H <sub>13</sub> N <sub>5</sub> O <sub>5</sub> •H <sub>2</sub> O	1.3139	C <sub>15</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub> •H <sub>2</sub> O
1.0194	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>6</sub>	1.3195	C <sub>13</sub> H <sub>20</sub> O <sub>2</sub> N <sub>2</sub> S•HCl•H <sub>2</sub> O
1.0194	C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O	1.3200	C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> •HCl•H <sub>2</sub> O
1.0410	C <sub>25</sub> H <sub>26</sub> O <sub>3</sub>	1.3219	C <sub>11</sub> H <sub>13</sub> N <sub>3</sub> O <sub>7</sub> (CH <sub>3</sub> C <sub>6</sub> ) <sub>2</sub> •HI•0.5CH <sub>3</sub> OH
1.0417	C <sub>20</sub> H <sub>30</sub> O <sub>2</sub> S	1.3257	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> •HCl•H <sub>2</sub> O
1.0445	C <sub>5</sub> H <sub>7</sub> O <sub>5</sub> (CH <sub>3</sub> ) <sub>3</sub>	1.3358	Ba(C <sub>3</sub> H <sub>6</sub> O <sub>7</sub> P) <sub>2</sub>
1.0570	C <sub>13</sub> H <sub>22</sub> O <sub>2</sub> N <sub>2</sub> S•HCl	1.3359	C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> O <sub>6</sub>
1.0576	C <sub>13</sub> H <sub>20</sub> O <sub>2</sub> N <sub>2</sub> S•HCl	1.3415	C <sub>6</sub> H <sub>3</sub> (NO <sub>2</sub> ) <sub>2</sub> •C <sub>6</sub> H <sub>5</sub> OC <sub>7</sub> H <sub>9</sub> -CH=CH-C <sub>10</sub> H <sub>15</sub> -CH(CH <sub>3</sub> ) CH=CHCH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>
1.0788	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>	1.3420	C <sub>12</sub> H <sub>24</sub> O <sub>7</sub>
1.0804	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>3</sub> •HP <sub>4</sub> •H <sub>2</sub> O	1.3423	C <sub>7</sub> H <sub>14</sub> O <sub>7</sub>
1.0822	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	1.3449	C <sub>14</sub> H <sub>15</sub> BrO <sub>7</sub>
1.0830	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> PS•IBr	1.3549	C <sub>18</sub> H <sub>20</sub> N <sub>3</sub> C <sub>2</sub> H <sub>5</sub> (OH) <sub>2</sub> (CH <sub>3</sub> ) <sub>4</sub> •HI•H <sub>2</sub> O
1.0830	C <sub>25</sub> H <sub>32</sub> BrN <sub>3</sub> O <sub>4</sub> •H <sub>2</sub> O	1.3602	C <sub>22</sub> H <sub>27</sub> O <sub>3</sub> N <sub>2</sub> Br•HBr
1.0888	C <sub>21</sub> H <sub>34</sub> O <sub>2</sub>	1.3606	C <sub>30</sub> H <sub>46</sub> O <sub>5</sub>
1.1011	C <sub>6</sub> H <sub>2</sub> (NO <sub>2</sub> ) <sub>3</sub> NHN(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •C <sub>6</sub> H <sub>6</sub>	1.3624	C <sub>22</sub> H <sub>27</sub> O <sub>3</sub> N <sub>2</sub> Br•HCl
1.1083	C <sub>23</sub> H <sub>17</sub> NO	1.3652	C <sub>32</sub> H <sub>48</sub> O <sub>6</sub>
1.1098	[(CH <sub>3</sub> ) <sub>3</sub> NCH <sub>2</sub> CH <sub>2</sub> OH]I	1.3655	(CH <sub>3</sub> ) <sub>3</sub> N <sub>3</sub> P <sub>3</sub> O <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub>
1.1209	C <sub>27</sub> H <sub>45</sub> I	1.3734	C <sub>16</sub> H <sub>18</sub> O <sub>4</sub> N <sub>2</sub> S•C <sub>13</sub> H <sub>20</sub> O <sub>2</sub> N <sub>2</sub> •H <sub>2</sub> O
1.1227	C <sub>26</sub> H <sub>31</sub> O <sub>3</sub> (C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> Cl)•H <sub>2</sub> O	1.3741	C <sub>41</sub> H <sub>58</sub> FeN <sub>9</sub> O <sub>20</sub> •4H <sub>2</sub> O
1.1245	[(CH <sub>3</sub> ) <sub>3</sub> As•PdClBr] <sub>2</sub>	1.3826	C <sub>6</sub> H <sub>11</sub> O <sub>9</sub> PA•7H <sub>2</sub> O
1.1294	C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> •2H <sub>2</sub> O	1.3826	CH <sub>3</sub> CH <sub>2</sub> O <sub>2</sub> C <sub>19</sub> H <sub>28</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>
1.1418	C <sub>26</sub> H <sub>34</sub> O <sub>7</sub>	1.3869	(CH <sub>3</sub> ) <sub>2</sub> CHCH(NH <sub>2</sub> )COOH•HBr
1.1426	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>	1.3881	C <sub>2</sub> HCl(C <sub>6</sub> H <sub>5</sub> NH <sub>4</sub> ) <sub>2</sub>
1.1439	C <sub>20</sub> H <sub>32</sub> O <sub>2</sub>	1.4032	C <sub>27</sub> H <sub>44</sub> O <sub>3</sub> Br
1.1468	Th(H <sub>2</sub> O) <sub>2</sub> (HC <sub>6</sub> H <sub>4</sub> ) <sub>4</sub> •H <sub>2</sub> O	1.4118	C <sub>20</sub> H <sub>26</sub> CuN <sub>4</sub> O <sub>2</sub> •2H <sub>2</sub> O
1.1486	C <sub>19</sub> H <sub>24</sub> O <sub>5</sub>	1.4161	C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O <sub>6</sub>
1.1508	C <sub>21</sub> H <sub>29</sub> BrN <sub>2</sub> S <sub>3</sub>	1.4225	C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub> S
1.1521	C <sub>28</sub> H <sub>42</sub> O <sub>3</sub>	1.4226	C <sub>27</sub> H <sub>45</sub> I
1.1568	C <sub>6</sub> H <sub>11</sub> O <sub>5</sub> •PF <sub>3</sub> K <sub>2</sub> •2H <sub>2</sub> O	1.4259	Cu(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> )Cl <sub>2</sub>
1.1575	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>	1.4282	C <sub>27</sub> H <sub>44</sub> ClBr
1.1597	C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub> •2HBr•2H <sub>2</sub> O	1.4345	C <sub>19</sub> H <sub>30</sub> O <sub>2</sub>
1.1608	C <sub>64</sub> H <sub>90</sub> N <sub>12</sub> O <sub>16</sub>	1.4366	C <sub>27</sub> H <sub>44</sub> Br <sub>2</sub>
1.1662	C <sub>6</sub> H <sub>3</sub> (NO <sub>2</sub> ) <sub>2</sub> •C <sub>6</sub> H <sub>5</sub> OC <sub>19</sub> H <sub>26</sub> -CH(CH <sub>3</sub> )CH•CHCH(CH <sub>3</sub> ) CH(CH <sub>3</sub> ) <sub>2</sub>	1.4373	(NH <sub>4</sub> ) <sub>2</sub> C <sub>4</sub> H <sub>4</sub> O <sub>6</sub>
1.1676	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>2</sub> •MnCl <sub>2</sub> •2H <sub>2</sub> O	1.4447	C <sub>19</sub> H <sub>34</sub>
1.1714	C <sub>6</sub> H <sub>13</sub> N <sub>7</sub> O <sub>7</sub> •H <sub>2</sub> O	1.4495	C <sub>19</sub> H <sub>14</sub> ClN <sub>6</sub> O <sub>9</sub> •C <sub>3</sub> H <sub>7</sub> NO
1.1739	C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> •HCl	1.4523	C <sub>18</sub> H <sub>32</sub>
1.1750	C <sub>20</sub> H <sub>30</sub> O <sub>2</sub>	1.4559	C <sub>19</sub> H <sub>14</sub> BrN <sub>6</sub> O <sub>9</sub> •C <sub>3</sub> H <sub>7</sub> NO
1.1816	C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> S	1.4571	2(C <sub>17</sub> H <sub>12</sub> O <sub>7</sub> )•C <sub>6</sub> H <sub>5</sub> Br
1.1833	CH <sub>3</sub> CH(NH <sub>2</sub> )CO <sub>2</sub> NHCH(CH <sub>3</sub> )CO <sub>2</sub> NHCH(CH <sub>3</sub> )CO <sub>2</sub> H	1.4661	(CH <sub>3</sub> ) <sub>2</sub> CHCH(NH <sub>2</sub> )COOH•HCl
1.1903	Be(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>2</sub>	1.4754	9CH <sub>4</sub> N <sub>2</sub> O•C <sub>8</sub> H <sub>14</sub> O <sub>4</sub>
1.2016	C <sub>10</sub> H <sub>15</sub> BrO	1.4799	C <sub>13</sub> H <sub>18</sub> ClHgO <sub>8</sub>
1.2032	C <sub>19</sub> H <sub>19</sub> N <sub>9</sub> O <sub>4</sub> •CH <sub>3</sub> I	1.4911	C <sub>19</sub> H <sub>30</sub> O <sub>2</sub>
1.2037	C <sub>10</sub> H <sub>15</sub> OCl	1.4911	C <sub>6</sub> H <sub>8</sub> O <sub>6</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>6</sub>
1.2049	C <sub>20</sub> H <sub>28</sub> O	1.4915	C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> •HBr•H <sub>2</sub> O
1.2098	C <sub>6</sub> H <sub>6</sub> (OH) <sub>5</sub> CH <sub>3</sub>	1.4937	C <sub>6</sub> H <sub>5</sub> •CH <sub>2</sub> •(C <sub>3</sub> H <sub>2</sub> N <sub>2</sub> )CHCOOH(CH <sub>3</sub> ) <sub>2</sub> SH•HCl
1.2103	C <sub>20</sub> H <sub>30</sub> O <sub>2</sub>	1.4938	2(C <sub>17</sub> H <sub>12</sub> O <sub>7</sub> )•C <sub>4</sub> H <sub>3</sub> SBr
1.2121	H <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> CH(NH <sub>2</sub> )COOH•HCl	1.5022	C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> •HCl•H <sub>2</sub> O
1.2233	C <sub>6</sub> H <sub>8</sub> O <sub>6</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>6</sub>	1.5043	2(C <sub>17</sub> H <sub>12</sub> O <sub>7</sub> )•C <sub>6</sub> H <sub>6</sub>
1.2288	C <sub>21</sub> H <sub>27</sub> N <sub>6</sub> O•HBr	1.5120	C <sub>9</sub> H <sub>7</sub> O <sub>10</sub> RbS
1.2516	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> •HCl	1.5177	C <sub>3</sub> H <sub>7</sub> N <sub>2</sub> O•HCl
1.2525	H <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> CH(NH <sub>2</sub> )COOH•HBr	1.5195	C <sub>23</sub> H <sub>36</sub> O <sub>2</sub>
1.2532	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	1.5244	C <sub>27</sub> H <sub>26</sub> O <sub>13</sub>
1.2545	C <sub>7</sub> H <sub>8</sub> O <sub>5</sub> (CH <sub>3</sub> ) <sub>2</sub>	1.5251	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>9</sub> •HBr•4H <sub>2</sub> O
1.2549	CaC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> •6H <sub>2</sub> O	1.5253	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>5</sub> •2H <sub>2</sub> O
1.2581	C <sub>27</sub> H <sub>46</sub> Cl <sub>2</sub>	1.5262	C <sub>34</sub> H <sub>18</sub>
1.2622	C <sub>46</sub> H <sub>66</sub> CoN <sub>11</sub> O <sub>9</sub> •11H <sub>2</sub> O	1.5329	C <sub>24</sub> H <sub>39</sub> NaO <sub>5</sub>
1.2631	C <sub>32</sub> H <sub>52</sub> INO <sub>3</sub>	1.5373	C <sub>14</sub> H <sub>10</sub>
1.2634	C <sub>10</sub> H <sub>15</sub> O•CN	1.5432	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>8</sub> Rb <sub>2</sub> •2H <sub>2</sub> O
1.2640	C <sub>21</sub> H <sub>28</sub> O <sub>3</sub> NI	1.5435	C <sub>14</sub> H <sub>25</sub> N <sub>3</sub> O <sub>9</sub> •HBr
1.2684	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> •HCl	1.5519	H <sub>2</sub> C <sub>19</sub> H <sub>29</sub> O <sub>9</sub>
1.2701	C <sub>28</sub> H <sub>46</sub> BrCl	1.5613	BaCa(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
1.2713	K(PtC <sub>2</sub> H <sub>4</sub> Cl <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> O	1.5640	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>9</sub> •HBr•2H <sub>2</sub> O
1.2729	C <sub>17</sub> H <sub>16</sub> BrClO <sub>6</sub>	1.5741	C <sub>10</sub> H <sub>16</sub> O <sub>2</sub>
1.2783	C <sub>6</sub> H <sub>11</sub> O <sub>5</sub> (CH <sub>3</sub> )	1.5789	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>9</sub> •HBr•2H <sub>2</sub> O
1.2805	C <sub>9</sub> H <sub>18</sub> INO <sub>6</sub>	1.5846	C <sub>20</sub> H <sub>33</sub> N <sub>3</sub> (HClO <sub>4</sub> ) <sub>2</sub>
1.2828	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> •HBr•H <sub>2</sub> O	1.5903	[C <sub>18</sub> H <sub>16</sub> HgN <sub>2</sub> O <sub>3</sub> S]
1.2867	C <sub>4</sub> H <sub>6</sub> O <sub>6</sub>	1.5917	NH <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> •CO <sub>2</sub> NH <sub>2</sub>
1.2888	C <sub>28</sub> H <sub>33</sub> O <sub>9</sub> I	1.6047	C <sub>32</sub> H <sub>53</sub> ClO <sub>2</sub>
1.2913	C <sub>21</sub> H <sub>36</sub> O <sub>3</sub>	1.6111	C <sub>27</sub> H <sub>44</sub> INO <sub>8</sub> •2H <sub>2</sub> O
1.2953	C <sub>7</sub> H <sub>13</sub> O <sub>6</sub> (CH <sub>3</sub> ) <sub>4</sub>	1.6133	C <sub>8</sub> H <sub>7</sub> NS <sub>2</sub>
1.2955	K(PtC <sub>2</sub> H <sub>4</sub> Br <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> O	1.6306	C <sub>23</sub> H <sub>29</sub> O <sub>2</sub> (OH)

P2<sub>1</sub> C<sub>2</sub><sup>2</sup> No. 4 (continued)

## Organic (continued)

1.6371	C <sub>21</sub> H <sub>32</sub> O <sub>3</sub>	2.0293	(C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> ) <sub>7</sub> ·xH <sub>2</sub> O
1.6467	C <sub>10</sub> H <sub>13</sub> O <sub>4</sub> Br	2.0363	Zn(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>2</sub> ·H <sub>2</sub> O
1.6495	(C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub> ) <sub>2</sub> ·H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> ·0.4(C <sub>4</sub> H <sub>7</sub> N <sub>2</sub> O <sub>4</sub> )·10H <sub>2</sub> O	2.0417	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>3</sub> ·H <sub>2</sub> O
1.6501	(C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub> ) <sub>2</sub> ·H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> ·12H <sub>2</sub> O	2.0464	C <sub>22</sub> H <sub>16</sub>
1.6514	(C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub> ) <sub>2</sub> ·H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> ·0.8(C <sub>4</sub> H <sub>4</sub> O <sub>4</sub> )·10H <sub>2</sub> O	2.0519	C <sub>19</sub> H <sub>30</sub> Cl-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>
1.6533	(C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub> ) <sub>2</sub> ·H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> ·CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> ·10H <sub>2</sub> O	2.0548	C <sub>10</sub> H <sub>15</sub> O <sub>2</sub> N·HBr
1.6552	(C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub> ) <sub>2</sub> ·H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> ·ClCH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> ·10H <sub>2</sub> O	2.0597	C <sub>10</sub> H <sub>15</sub> O <sub>4</sub> N
1.6571	(C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub> ) <sub>2</sub> ·H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> ·CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> ·10H <sub>2</sub> O	2.0620	CH <sub>3</sub> C <sub>19</sub> H <sub>28</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>
1.6587	(C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub> ) <sub>2</sub> ·H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> ·C <sub>2</sub> H <sub>5</sub> C <sub>6</sub> H <sub>4</sub> ·10H <sub>2</sub> O	2.0669	C <sub>19</sub> H <sub>31</sub> O <sub>2</sub> N·HBr·CH <sub>3</sub> OH
1.6610	(C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub> ) <sub>2</sub> ·H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> ·C <sub>2</sub> H <sub>5</sub> O <sub>4</sub> ·10H <sub>2</sub> O	2.0670	C <sub>32</sub> H <sub>49</sub> N <sub>2</sub> O <sub>5</sub> ·HBr
1.6614	C <sub>19</sub> H <sub>32</sub> O <sub>2</sub>	2.0772	C <sub>6</sub> H <sub>5</sub> CH(OH)CH(CH <sub>3</sub> )NHCH <sub>3</sub> ·HCl
1.6622	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>	2.0862	C <sub>19</sub> H <sub>31</sub> N <sub>2</sub> O <sub>2</sub> ·HCl·CH <sub>3</sub> OH
1.6642	C <sub>32</sub> H <sub>53</sub> I <sub>2</sub>	2.0961	(C <sub>10</sub> H <sub>13</sub> N <sub>2</sub> O <sub>8</sub> P)Ca·6H <sub>2</sub> O
1.6644	(C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub> ) <sub>2</sub> ·H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> ·BrCH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> ·10H <sub>2</sub> O	2.1125	(CH <sub>3</sub> ) <sub>2</sub> CH·CH <sub>2</sub> ·CH(NH <sub>2</sub> )C <sub>6</sub> H <sub>4</sub> ·CH <sub>2</sub> ·C <sub>6</sub> H <sub>4</sub>
1.6667	(C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub> ) <sub>2</sub> ·H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> ·C <sub>3</sub> H <sub>4</sub> O <sub>4</sub> ·10H <sub>2</sub> O	2.1160	CH <sub>3</sub> C <sub>19</sub> H <sub>28</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>
1.6672	NH <sub>2</sub> ·CH <sub>2</sub> ·C <sub>6</sub> H <sub>4</sub> ·NH·CH <sub>2</sub> ·CH <sub>3</sub> ·C <sub>6</sub> H <sub>4</sub>	2.1216	C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> ·HCl
1.6680	C <sub>19</sub> H <sub>25</sub> -CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>	2.1254	C <sub>7</sub> H <sub>10</sub> O <sub>5</sub> ·Sr·4H <sub>2</sub> O
1.6683	(C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub> ) <sub>2</sub> ·H <sub>2</sub> SiF <sub>6</sub> ·ClCH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> ·10H <sub>2</sub> O	2.1258	C <sub>19</sub> H <sub>28</sub> Br-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>
1.6740	C <sub>27</sub> H <sub>37</sub> N <sub>2</sub> O <sub>7</sub> ·HBr	2.1419	C <sub>27</sub> H <sub>39</sub> O <sub>3</sub> N·HBr
1.6786	C <sub>10</sub> H <sub>15</sub> O <sub>2</sub> N·C <sub>4</sub> H <sub>6</sub> O <sub>6</sub> ·H <sub>2</sub> O	2.1556	C <sub>8</sub> H <sub>20</sub> N <sub>2</sub> O <sub>6</sub> P
1.6786	C <sub>5</sub> H <sub>9</sub> O <sub>5</sub> CH <sub>3</sub>	2.1612	C <sub>12</sub> H <sub>16</sub> O <sub>3</sub>
1.6863	C <sub>6</sub> H <sub>2</sub> CHCl(N <sub>2</sub> ) <sub>2</sub>	2.1625	C <sub>27</sub> H <sub>45</sub> Cl
1.7088	C <sub>27</sub> H <sub>46</sub> O	2.1734	C <sub>23</sub> H <sub>32</sub> O <sub>7</sub>
1.7182	C <sub>19</sub> H <sub>32</sub> O <sub>2</sub>	2.1822	C <sub>23</sub> H <sub>32</sub> O <sub>6</sub>
1.7300	C <sub>23</sub> H <sub>32</sub> O <sub>3</sub>	2.1884	C <sub>6</sub> H <sub>5</sub> -CH(OH)-CH(OH)-C <sub>6</sub> H <sub>5</sub>
1.7311	C <sub>14</sub> H <sub>12</sub>	2.1912	C <sub>6</sub> H <sub>5</sub> -CH(OH)-CH(OH)-C <sub>6</sub> H <sub>5</sub>
1.7360	C <sub>20</sub> H <sub>28</sub> O <sub>3</sub>	2.1984	C <sub>23</sub> H <sub>30</sub> O <sub>6</sub> ·2H <sub>2</sub> O
1.7401	C <sub>6</sub> H <sub>11</sub> N <sub>2</sub> O <sub>2</sub> ·HBr	2.1987	C <sub>19</sub> H <sub>28</sub> Cl-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>
1.7439	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> ·HBr·H <sub>2</sub> O	2.2022	C <sub>21</sub> H <sub>30</sub> O <sub>5</sub>
1.7527	C <sub>15</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>	2.2026	CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> -C <sub>19</sub> H <sub>30</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>
1.7585	C <sub>22</sub> H <sub>25</sub> Cl <sub>4</sub> Fe <sub>2</sub> O <sub>6</sub>	2.2117	(CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub> C <sub>5</sub> H <sub>7</sub> O <sub>4</sub> (C <sub>6</sub> H <sub>4</sub> N <sub>4</sub> O <sub>4</sub> )
1.7587	C <sub>27</sub> H <sub>48</sub>	2.2140	C <sub>19</sub> H <sub>28</sub> Cl-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> ·HCl
1.7631	C <sub>15</sub> H <sub>22</sub> O <sub>4</sub>	2.2384	C <sub>5</sub> H <sub>6</sub> O <sub>5</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub>
1.7759	H <sub>2</sub> NCH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> NH·CH(CH <sub>3</sub> )C <sub>6</sub> H <sub>4</sub> ·HCl·H <sub>2</sub> O	2.2628	C <sub>30</sub> H <sub>46</sub> O <sub>4</sub>
1.7819	C <sub>11</sub> H <sub>7</sub> Cl <sub>2</sub> O <sub>2</sub>	2.2707	(CH <sub>3</sub> ) <sub>2</sub> CHCHNH <sub>2</sub> C <sub>6</sub> H <sub>4</sub>
1.7861	C <sub>9</sub> H <sub>9</sub> N <sub>2</sub> O <sub>4</sub> I	2.2762	C <sub>25</sub> H <sub>20</sub>
1.7891	C <sub>24</sub> H <sub>40</sub> O <sub>5</sub> ·4H <sub>2</sub> O	2.2781	C <sub>10</sub> H <sub>16</sub> O <sub>2</sub>
1.7990	C <sub>13</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub> ·2H <sub>2</sub> O	2.2815	C <sub>20</sub> H <sub>25</sub> N <sub>3</sub> O <sub>4</sub> S·HBr·H <sub>2</sub> O
1.8000	C <sub>19</sub> H <sub>31</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>	2.2818	C <sub>9</sub> H <sub>11</sub> BrN <sub>2</sub> O <sub>6</sub>
1.8003	C <sub>13</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub> ·H <sub>2</sub> O	2.2911	C <sub>11</sub> H <sub>15</sub> BrN <sub>2</sub> O <sub>4</sub>
1.8061	C <sub>22</sub> H <sub>14</sub>	2.3207	C <sub>30</sub> H <sub>52</sub> O
1.8220	C <sub>8</sub> H <sub>12</sub> O <sub>2</sub>	2.3340	C <sub>8</sub> H <sub>15</sub> N <sub>2</sub> O <sub>6</sub>
1.8303	(CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub> C <sub>5</sub> H <sub>7</sub> O <sub>4</sub> (C <sub>6</sub> H <sub>4</sub> N <sub>4</sub> O <sub>4</sub> )	2.3388	C <sub>21</sub> H <sub>32</sub> O <sub>3</sub>
1.8524	C <sub>19</sub> H <sub>27</sub> O-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>	2.3513	C <sub>29</sub> H <sub>45</sub> Br <sub>2</sub> O <sub>4</sub>
1.8545	C <sub>23</sub> H <sub>34</sub> O <sub>4</sub>	2.3546	C <sub>12</sub> H <sub>12</sub> BrN <sub>2</sub> O <sub>8</sub> S
1.8619	C <sub>27</sub> H <sub>43</sub> O <sub>3</sub> ·C <sub>6</sub> H <sub>5</sub> ·CH <sub>3</sub>	2.3547	C <sub>9</sub> H <sub>11</sub> BrN <sub>2</sub> O <sub>5</sub>
1.8628	C <sub>27</sub> H <sub>44</sub> O	2.3571	C <sub>19</sub> H <sub>30</sub> O <sub>2</sub> H-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>
1.8646	C <sub>18</sub> H <sub>12</sub>	2.3585	C <sub>24</sub> H <sub>18</sub>
1.8755	C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> O <sub>7</sub> P·2H <sub>2</sub> O	2.3631	C <sub>29</sub> H <sub>45</sub> I <sub>2</sub> O <sub>4</sub>
1.8794	C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> O <sub>7</sub> P·1.5H <sub>2</sub> O	2.3651	C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
1.8852	(NH <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>4</sub> Br	2.3693	C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O·HCl
1.8872	(C <sub>4</sub> H <sub>8</sub> )(C <sub>6</sub> H <sub>5</sub> CHCH <sub>3</sub> NH <sub>2</sub> )PtCl <sub>2</sub>	2.3763	C <sub>10</sub> H <sub>22</sub> O <sub>5</sub> S <sub>2</sub>
1.8876	C <sub>25</sub> H <sub>40</sub> N <sub>2</sub> O <sub>2</sub> ·H <sub>2</sub> O	2.4024	C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O·HBr
1.8923	C <sub>27</sub> H <sub>44</sub> O <sub>2</sub> ·H <sub>2</sub> O	2.4196	(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> O <sub>2</sub> H
1.8974	C <sub>19</sub> H <sub>30</sub> Cl-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>	2.4303	C <sub>20</sub> H <sub>30</sub> O <sub>5</sub>
1.8990	Cu(C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> ) <sub>2</sub>	2.4433	C <sub>11</sub> H <sub>8</sub> O <sub>3</sub>
1.9000	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> ·H <sub>2</sub> O	2.4492	C <sub>10</sub> H <sub>19</sub> O <sub>3</sub> S <sub>2</sub> ·C <sub>6</sub> H <sub>4</sub> I
1.9050	CH <sub>3</sub> ·C <sub>6</sub> H <sub>4</sub> ·C <sub>19</sub> H <sub>30</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>	2.4548	C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> S <sub>2</sub>
1.9066	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> ·H <sub>2</sub> O	2.4593	OH·C <sub>6</sub> H <sub>4</sub> ·CH <sub>2</sub> ·CH(OH)·(NH <sub>2</sub> ·HCl)·C <sub>6</sub> H <sub>4</sub>
1.9071	C <sub>21</sub> H <sub>28</sub> O <sub>4</sub>	2.4597	C <sub>28</sub> H <sub>46</sub> Cl <sub>2</sub>
1.9196	C <sub>9</sub> H <sub>14</sub> N <sub>3</sub> O <sub>7</sub> P	2.4605	C <sub>15</sub> H <sub>16</sub> O <sub>2</sub>
1.9225	C <sub>27</sub> H <sub>46</sub> Cl <sub>2</sub>	2.4692	C <sub>16</sub> H <sub>17</sub> N <sub>2</sub> O <sub>4</sub> S·Na
1.9366	C <sub>27</sub> H <sub>44</sub> O <sub>4</sub>	2.4740	C <sub>29</sub> H <sub>44</sub> Br <sub>2</sub> O <sub>4</sub>
1.9369	C <sub>27</sub> H <sub>46</sub> Br <sub>2</sub>	2.4787	C <sub>29</sub> H <sub>45</sub> Br <sub>2</sub> O <sub>4</sub>
1.9447	C <sub>19</sub> H <sub>29</sub> Cl <sub>2</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>	2.4821	C <sub>32</sub> H <sub>39</sub> Br <sub>2</sub> O <sub>11</sub>
1.9478	C <sub>19</sub> H <sub>29</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>	2.5008	C <sub>19</sub> H <sub>28</sub> O <sub>2</sub> H-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> ·H <sub>2</sub> O
1.9647	C <sub>8</sub> H <sub>16</sub> O <sub>5</sub> S	2.5306	C <sub>29</sub> H <sub>46</sub> O <sub>4</sub>
1.9744	C <sub>13</sub> H <sub>15</sub> N <sub>2</sub> O <sub>2</sub> ·HBr·2H <sub>2</sub> O	2.5314	C <sub>29</sub> H <sub>44</sub> Br <sub>2</sub> O <sub>4</sub>
1.9775	(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>2</sub> Zn·H <sub>2</sub> O	2.5437	C <sub>24</sub> H <sub>32</sub> O <sub>4</sub>
1.9867	C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> ·HBr	2.5754	(CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> S) <sub>2</sub>
1.9899	C <sub>27</sub> H <sub>39</sub> O <sub>3</sub> N·HI	2.5890	C <sub>6</sub> H <sub>5</sub> -CH(OH)(C <sub>6</sub> H <sub>4</sub> )
2.0059	C <sub>10</sub> H <sub>7</sub> HgI	2.6104	C <sub>19</sub> H <sub>26</sub> O <sub>2</sub> H-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>
2.0066	C <sub>5</sub> H <sub>11</sub> O <sub>2</sub> NS·HCl·H <sub>2</sub> O	2.6213	C <sub>31</sub> H <sub>43</sub> I <sub>2</sub> O <sub>5</sub>
2.0154	C <sub>19</sub> H <sub>31</sub> N <sub>2</sub> O <sub>2</sub> ·HI·CH <sub>3</sub> OH		

P<sub>21</sub> C<sub>2</sub><sup>2</sup> No. 4 (continued)

## Organic (continued)

2.6240	CH <sub>3</sub> •Cθ•θ-C <sub>19</sub> H <sub>26</sub> (C <sub>4</sub> H <sub>2</sub> θ <sub>3</sub> )-CH(CH <sub>3</sub> )CH(Br)CH(Br) CH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>	4.0185	C <sub>14</sub> H <sub>7</sub> Iθ <sub>2</sub>
2.6765	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> θ <sub>2</sub> •HBr	4.0461	C <sub>19</sub> H <sub>26</sub> (θH) <sub>3</sub> -CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub> •2H <sub>2</sub> θ
2.6766	C <sub>6</sub> H <sub>8</sub> θ <sub>6</sub>	4.0708	CH <sub>3</sub> •Cθ•θ•C <sub>19</sub> H <sub>26</sub> (C <sub>4</sub> H <sub>2</sub> θ <sub>3</sub> )-CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> ) CH(CH <sub>3</sub> ) <sub>2</sub>
2.6950	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> θ <sub>2</sub> •HBr	4.2333	C <sub>14</sub> H <sub>7</sub> Brθ <sub>2</sub>
2.6959	C <sub>35</sub> H <sub>46</sub> Iθ <sub>4</sub>	4.2832	C <sub>14</sub> H <sub>7</sub> Clθ <sub>2</sub>
2.7451	C <sub>16</sub> H <sub>29</sub> θ <sub>4</sub> •Sθ <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> Br	4.2954	C <sub>19</sub> H <sub>38</sub> θ <sub>2</sub>
2.7473	C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> θ <sub>3</sub>	4.4400	C <sub>19</sub> H <sub>28</sub> (θH) <sub>3</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>
2.7679	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> θ <sub>2</sub> •HCl	4.5135	C <sub>32</sub> H <sub>53</sub> Brθ <sub>4</sub>
2.7797	C <sub>23</sub> H <sub>30</sub> θ <sub>3</sub>	4.5207	HθC <sub>7</sub> H <sub>10</sub> -CH <sub>2</sub> CH=C <sub>10</sub> H <sub>15</sub> -CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> ) CH(CH <sub>3</sub> ) <sub>2</sub>
2.8000	C <sub>19</sub> H <sub>26</sub> θH-CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>	4.5396	C <sub>19</sub> H <sub>26</sub> (θH) <sub>3</sub> -CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>
2.8593	C <sub>35</sub> H <sub>47</sub> θ <sub>2</sub> Br	4.5910	CH <sub>3</sub> •Cθ•θ•C <sub>19</sub> H <sub>26</sub> -CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>
2.8671	C <sub>19</sub> H <sub>26</sub> θH-CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>	4.6328	C <sub>19</sub> H <sub>26</sub> θH-CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> θ
2.8712	(Nθ <sub>2</sub> )C <sub>6</sub> H <sub>4</sub> CHθ	4.6424	C <sub>19</sub> H <sub>28</sub> θH-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH(C <sub>2</sub> H <sub>5</sub> )CH(CH <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> θ
2.9195	CH <sub>3</sub> •Cθ•θ•C <sub>19</sub> H <sub>26</sub> -CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>	4.7785	CH <sub>3</sub> •Cθ•θ•C <sub>19</sub> H <sub>28</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH(C <sub>2</sub> H <sub>5</sub> ) CH(CH <sub>3</sub> ) <sub>2</sub>
3.0562	C <sub>32</sub> H <sub>52</sub> θ <sub>2</sub>	4.8432	C <sub>19</sub> H <sub>28</sub> θH-CH(CH <sub>3</sub> )CH=CHCH(C <sub>2</sub> H <sub>5</sub> )CH(CH <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> θ
3.0685	C <sub>34</sub> H <sub>39</sub> Iθ <sub>10</sub>	4.8797	C <sub>19</sub> H <sub>26</sub> θHθ-θ-CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>
3.0856	C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> θ <sub>5</sub>	4.9444	HθC <sub>7</sub> H <sub>9</sub> =CHCH=C <sub>10</sub> H <sub>15</sub> -CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> ) CH(CH <sub>3</sub> ) <sub>2</sub>
3.1420	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> θ <sub>5</sub>	5.0525	C <sub>19</sub> H <sub>28</sub> θH-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH(C <sub>2</sub> H <sub>5</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>
3.2245	C <sub>18</sub> H <sub>13</sub> As	5.0606	C <sub>14</sub> H <sub>27</sub> Brθ <sub>4</sub>
3.3997	C <sub>20</sub> H <sub>21</sub> Brθ <sub>6</sub>	5.0682	C <sub>8</sub> H <sub>10</sub> θ
3.3997	C <sub>20</sub> H <sub>21</sub> Brθ <sub>6</sub>	5.0911	C <sub>19</sub> H <sub>12</sub> θ <sub>2</sub>
3.4860	Cu(SCN) <sub>2</sub> •2C <sub>5</sub> H <sub>5</sub> N	5.1381	C <sub>15</sub> H <sub>12</sub> θ <sub>4</sub> NI <sub>3</sub> •HCl
3.5346	C <sub>23</sub> H <sub>30</sub> θ <sub>6</sub>	5.1701	C <sub>19</sub> H <sub>28</sub> θH-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>
3.5599	C <sub>23</sub> H <sub>36</sub> θ <sub>3</sub>	5.1939	C <sub>45</sub> H <sub>80</sub> θ <sub>2</sub>
3.5930	C <sub>19</sub> H <sub>31</sub> •C <sub>2</sub> H <sub>5</sub>	5.8205	C <sub>29</sub> H <sub>43</sub> Iθ <sub>4</sub>
3.6153	C <sub>39</sub> H <sub>68</sub> θ <sub>2</sub>	5.8361	C <sub>19</sub> H <sub>28</sub> θH-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>
3.6312	C <sub>6</sub> H <sub>5</sub> NH-N=C <sub>6</sub> H <sub>5</sub>	6.0170	C <sub>36</sub> H <sub>72</sub> Nθ <sub>8</sub> P
3.6462	C <sub>23</sub> H <sub>20</sub> θ <sub>10</sub>		
3.6885	C <sub>17</sub> H <sub>18</sub> Br <sub>2</sub> N <sub>4</sub> θ <sub>3</sub>		
3.8799	C <sub>29</sub> H <sub>28</sub> Br <sub>2</sub> θ <sub>6</sub>		
3.9774	C <sub>17</sub> H <sub>18</sub> Br <sub>2</sub> N <sub>4</sub> θ <sub>3</sub>		
4.0000	(C <sub>20</sub> H <sub>24</sub> θ <sub>2</sub> N <sub>2</sub> ) <sub>2</sub> H <sub>2</sub> Sθ <sub>4</sub> •2H <sub>2</sub> θ		

2

C<sub>2</sub> C<sub>2</sub><sup>3</sup> No. 5Inorganic - 78  
Organic - 80

## Inorganic

0.4436	BiVθ <sub>4</sub>	0.4888	AmTaθ <sub>4</sub>
0.4758	YTi <sub>0.5</sub> W <sub>0.5</sub> θ <sub>4</sub>	0.4889	EuTaθ <sub>4</sub>
0.4780	LuTi <sub>0.5</sub> W <sub>0.5</sub> θ <sub>4</sub>	0.4898	SmTaθ <sub>4</sub>
0.4810	YTaθ <sub>4</sub>	0.4907	NdTaθ <sub>4</sub>
0.4812	LuTaθ <sub>4</sub>	1.0275	Na <sub>2</sub> ZrSi <sub>6</sub> θ <sub>15</sub> •3H <sub>2</sub> θ•0.5NaθH
0.4815	YbTi <sub>0.5</sub> W <sub>0.5</sub> θ <sub>4</sub>	1.0704	K <sub>2</sub> MoθF <sub>5</sub> •H <sub>2</sub> θ
0.4827	LaNbθ <sub>4</sub>	1.0709	LiFeSi <sub>2</sub> θ <sub>6</sub>
0.4830	ImTi <sub>0.5</sub> W <sub>0.5</sub> θ <sub>4</sub>	1.0838	LiAlSi <sub>2</sub> θ <sub>6</sub>
0.4830	YbNbθ <sub>4</sub>	1.1208	In(θH)F <sub>2</sub>
0.4831	CmNbθ <sub>4</sub>	1.3319	As(CN) <sub>3</sub>
0.4832	LuNbθ <sub>4</sub>	1.5323	Mθ <sub>6</sub> (θH) <sub>6</sub> (Si,Al) <sub>4</sub> θ <sub>10</sub>
0.4835	HoNbθ <sub>4</sub>	1.5430	[Ru(NH <sub>3</sub> ) <sub>4</sub> (Nθ)(θH)]Cl <sub>2</sub>
0.4836	DyNbθ <sub>4</sub>	1.6575	Ca <sub>3</sub> V <sub>10</sub> θ <sub>28</sub> •17H <sub>2</sub> θ
0.4837	YNbθ <sub>4</sub>	1.7909	Na <sub>2</sub> Al <sub>2</sub> Si <sub>3</sub> θ <sub>10</sub>
0.4837	ErNbθ <sub>4</sub>	1.8594	CaSθ <sub>4</sub> •0.5H <sub>2</sub> θ
0.4838	TmNbθ <sub>4</sub>	1.9803	Na <sub>2</sub> Al <sub>2</sub> Si <sub>3</sub> θ <sub>10</sub> •2H <sub>2</sub> θ
0.4840	(Y, Yb)Nbθ <sub>4</sub>	1.9943	Pb(N <sub>3</sub> ) <sub>2</sub>
0.4843	GdNbθ <sub>4</sub>	2.2057	Na <sub>2</sub> S <sub>4</sub> θ <sub>6</sub> •2H <sub>2</sub> θ
0.4844	AmNbθ <sub>4</sub>	2.5534	P <sub>2</sub> Ta
0.4844	EuNbθ <sub>4</sub>	2.5587	P <sub>2</sub> W
0.4845	PuNbθ <sub>4</sub>	2.5624	P <sub>2</sub> W
0.4847	NdNbθ <sub>4</sub>	2.5659	Sb <sub>2</sub> Ta
0.4847	TbNbθ <sub>4</sub>	2.5682	NbP <sub>2</sub>
0.4848	PrNbθ <sub>4</sub>	2.5685	As <sub>2</sub> Ta
0.4851	SmNbθ <sub>4</sub>	2.5695	NbP <sub>2</sub>
0.4852	CeNbθ <sub>4</sub>	2.5700	As <sub>2</sub> V
0.4862	PrNbθ <sub>4</sub>	2.5702	P <sub>2</sub> V
0.4870	CmTaθ <sub>4</sub>	2.5720	As <sub>2</sub> W
0.4871	ErTaθ <sub>4</sub>	2.5866	As <sub>2</sub> Nb
0.4873	HoTaθ <sub>4</sub>	2.5928	As <sub>2</sub> Mo
0.4879	DyTaθ <sub>4</sub>	2.5943	NbSb <sub>2</sub>
0.4883	TbTaθ <sub>4</sub>	2.5945	As <sub>2</sub> Mo
0.4886	GdTaθ <sub>4</sub>	2.8513	As <sub>2</sub> Mo

C2 C<sub>2</sub><sup>3</sup> No. 5 (continued)

## Inorganic (continued)

3.2571 GaNb<sub>4</sub>  
 3.2867 Po  
 3.3267 KAl<sub>2</sub>Si<sub>4</sub>Cl<sub>10</sub>(OH)<sub>2</sub>  
 3.4257 K(SeCN)<sub>3</sub>•0.5H<sub>2</sub>O  
 5.0722 WNb<sub>12</sub>Cl<sub>33</sub>  
 5.2571 Mg<sub>2</sub>(OH)<sub>2</sub>Cl<sub>3</sub>•3H<sub>2</sub>O

5.3453 V<sub>2</sub>Mo<sub>6</sub>  
 6.4058 W<sub>5</sub>Nb<sub>16</sub>Cl<sub>55</sub>  
 7.7772 W<sub>4</sub>Nb<sub>26</sub>Cl<sub>77</sub>  
 7.7538 TiNb<sub>24</sub>Cl<sub>62</sub>  
 8.6697 Ca<sub>2</sub>Nb<sub>2</sub>(Al<sub>2</sub>Si<sub>3</sub>Cl<sub>10</sub>)<sub>3</sub>•8H<sub>2</sub>O  
 9.7965 Nb<sub>31</sub>Cl<sub>77</sub>F

## Organic

0.2440 C<sub>6</sub>H<sub>5</sub>BrHg  
 0.7517 C<sub>21</sub>H<sub>12</sub>Cl<sub>2</sub>CuN<sub>4</sub>  
 0.8876 C<sub>6</sub>H<sub>5</sub>CC<sub>6</sub>H<sub>5</sub>•GeBr<sub>2</sub>  
 1.0448 C<sub>6</sub>H<sub>8</sub>Cl<sub>2</sub>S<sub>2</sub>•C<sub>6</sub>H<sub>8</sub>Cl<sub>2</sub>Se<sub>2</sub>  
 1.1368 C<sub>6</sub>H<sub>5</sub>CC<sub>6</sub>H<sub>5</sub>•GeCl<sub>2</sub>  
 1.1917 C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>Cl<sub>5</sub>S  
 1.2947 (NH<sub>4</sub>)<sub>2</sub>[(MoCl<sub>3</sub>)<sub>2</sub>C<sub>4</sub>H<sub>4</sub>Cl<sub>5</sub>]•2.5H<sub>2</sub>O  
 1.3319 As(CN)<sub>3</sub>  
 1.4550 (AgClCC<sub>3</sub>F<sub>7</sub>)<sub>2</sub>  
 1.5319 C<sub>29</sub>H<sub>45</sub>Br<sub>4</sub>  
 1.5405 Ca(C<sub>6</sub>H<sub>9</sub>Cl<sub>7</sub>)<sub>2</sub>•2H<sub>2</sub>O  
 1.5941 (C<sub>6</sub>H<sub>12</sub>Cl<sub>6</sub>)<sub>2</sub>•SrCl<sub>2</sub>•3H<sub>2</sub>O  
 1.6294 C<sub>19</sub>H<sub>30</sub>OH-CH(CH<sub>3</sub>)(CH<sub>2</sub>)<sub>3</sub>CH(CH<sub>3</sub>)<sub>2</sub>•C<sub>2</sub>H<sub>5</sub>OH  
 1.7033 C<sub>5</sub>H<sub>9</sub>Cl<sub>5</sub>•P<sub>2</sub>Cl<sub>3</sub>•Ba•5H<sub>2</sub>O  
 1.7595 C<sub>20</sub>H<sub>26</sub>Cl<sub>4</sub>N<sub>2</sub>•CH<sub>3</sub>I  
 1.8649 (Mg<sub>2</sub>.88Al<sub>0.12</sub>)(Si<sub>2.84</sub>Al<sub>1.16</sub>)Cl<sub>10</sub>  
 (OH)<sub>2</sub>•[(NH<sub>2</sub>(CH<sub>2</sub>)<sub>6</sub>NH<sub>3</sub>)<sub>0.5</sub>Na<sub>0.5</sub>]  
 1.9101 (C<sub>18</sub>H<sub>28</sub>N<sub>6</sub>)<sub>2</sub>PtCl<sub>6</sub>•2H<sub>2</sub>O  
 1.9343 (CH<sub>3</sub>)<sub>3</sub>N(I)(CH<sub>2</sub>)<sub>2</sub>Cl<sub>2</sub>•CH<sub>3</sub>  
 2.2564 C<sub>18</sub>H<sub>24</sub>Cl<sub>2</sub>  
 2.3908 C<sub>22</sub>H<sub>22</sub>BrN<sub>3</sub>Cl<sub>8</sub>S•0.5C<sub>6</sub>H<sub>6</sub>  
 2.4562 C<sub>66</sub>H<sub>60</sub>Br<sub>2</sub>Cl<sub>12</sub>•2C<sub>6</sub>H<sub>6</sub>  
 2.5310 K<sub>2</sub>[ClC(CH<sub>3</sub>)<sub>2</sub>Cl]•0.5H<sub>2</sub>O  
 2.5326 Ca(ClCC[CH<sub>3</sub>CH<sub>2</sub>OH])<sub>3</sub>•5H<sub>2</sub>O  
 2.5369 Sr[ClCC[CH<sub>3</sub>CH<sub>2</sub>OH])<sub>3</sub>•5H<sub>2</sub>O  
 2.6162 C<sub>23</sub>H<sub>34</sub>Cl<sub>4</sub>  
 2.6281 [Co(NH<sub>2</sub>CH<sub>2</sub>CH(CH<sub>3</sub>)NH<sub>2</sub>)<sub>2</sub>Cl<sub>2</sub>]Cl•HCl•2H<sub>2</sub>O  
 2.7216 C<sub>25</sub>H<sub>42</sub>Cl<sub>5</sub>•C<sub>2</sub>H<sub>5</sub>OH  
 2.8841 Zn(C<sub>7</sub>H<sub>5</sub>Cl<sub>3</sub>)<sub>2</sub>•2H<sub>2</sub>O  
 2.9703 (C<sub>20</sub>H<sub>24</sub>N<sub>2</sub>Cl<sub>2</sub>)<sub>2</sub>•H<sub>2</sub>SeCl<sub>4</sub>•2H<sub>2</sub>O  
 2.9703 (C<sub>20</sub>H<sub>24</sub>N<sub>2</sub>Cl<sub>2</sub>)<sub>2</sub>•H<sub>2</sub>SeCl<sub>4</sub>•2H<sub>2</sub>O  
 2.9752 C<sub>10</sub>H<sub>18</sub>N<sub>4</sub>Cl<sub>6</sub>S<sub>2</sub>•2H<sub>2</sub>O  
 3.0039 C<sub>34</sub>H<sub>28</sub>Br<sub>2</sub>Cl<sub>8</sub>  
 3.0127 C<sub>22</sub>H<sub>26</sub>N<sub>2</sub>Cl<sub>3</sub>  
 3.0432 C<sub>16</sub>H<sub>18</sub>N<sub>2</sub>Cl<sub>4</sub>S  
 3.1328 C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>Cl<sub>3</sub>•0.5NaI  
 3.2421 CH<sub>3</sub>•C<sub>6</sub>H<sub>4</sub>•C<sub>19</sub>H<sub>26</sub>(C<sub>4</sub>H<sub>2</sub>Cl<sub>3</sub>)-CH(CH<sub>3</sub>)  
 CH=CHCH(CH<sub>3</sub>)CH(CH<sub>3</sub>)<sub>2</sub>  
 3.3238 C<sub>19</sub>H<sub>26</sub>(OH)<sub>3</sub>-CH(CH<sub>3</sub>)CH=CHCH(CH<sub>3</sub>)CH(CH<sub>3</sub>)<sub>2</sub>  
 3.3492 NaCl•ClC(NH<sub>2</sub>)<sub>2</sub>•H<sub>2</sub>O  
 3.4257 K(SeCN)<sub>3</sub>•0.5H<sub>2</sub>O

3.4492 C<sub>19</sub>H<sub>28</sub>Cl<sub>2</sub>  
 3.4876 (H<sub>2</sub>CC•CH(NH<sub>3</sub>Cl)CH<sub>2</sub>S)<sub>2</sub>  
 3.4925 C<sub>23</sub>H<sub>23</sub>I<sub>8</sub>  
 3.5385 Co(C<sub>6</sub>H<sub>8</sub>N<sub>3</sub>Cl<sub>2</sub>)<sub>2</sub>•H<sub>2</sub>O  
 3.6267 C<sub>28</sub>H<sub>43</sub>Cl<sub>8</sub>  
 3.7617 [NH<sub>2</sub>(CH<sub>3</sub>)C<sub>6</sub>H<sub>3</sub>]<sub>2</sub>•2HCl  
 3.7853 C<sub>35</sub>H<sub>46</sub>IN<sub>4</sub>  
 3.9699 C<sub>23</sub>H<sub>31</sub>Cl<sub>2</sub>(OH)<sub>3</sub>  
 4.0055 C<sub>21</sub>H<sub>36</sub>Cl<sub>2</sub>  
 4.1519 C<sub>30</sub>H<sub>44</sub>Br<sub>2</sub>Cl<sub>2</sub>  
 4.1854 C<sub>6</sub>H<sub>4</sub>(Cl)<sub>2</sub>N(CH<sub>2</sub>)<sub>10</sub>N(CH<sub>3</sub>)<sub>3</sub>I  
 4.1959 C<sub>19</sub>H<sub>26</sub>OH-CH(CH<sub>3</sub>)CH=CHCH(CH<sub>3</sub>)CH(CH<sub>3</sub>)<sub>2</sub>  
 4.3549 CH<sub>3</sub>•C<sub>6</sub>H<sub>4</sub>•C<sub>19</sub>H<sub>28</sub>-CH(CH<sub>3</sub>)CH<sub>2</sub>CH<sub>2</sub>CH(CH<sub>3</sub>)CH(CH<sub>3</sub>)<sub>2</sub>  
 4.5303 (C<sub>21</sub>H<sub>22</sub>N<sub>2</sub>Cl<sub>2</sub>)<sub>2</sub>•H<sub>2</sub>SeCl<sub>4</sub>•5H<sub>2</sub>O  
 4.5423 (C<sub>21</sub>H<sub>22</sub>N<sub>2</sub>Cl<sub>2</sub>)<sub>2</sub>•H<sub>2</sub>SeCl<sub>4</sub>•5H<sub>2</sub>O  
 4.5606 C<sub>24</sub>H<sub>42</sub>Cl<sub>4</sub>  
 4.5800 CH<sub>3</sub>•C<sub>6</sub>H<sub>4</sub>•C<sub>19</sub>H<sub>28</sub>-CH(CH<sub>3</sub>)CH=CHCH(CH<sub>2</sub>H<sub>5</sub>)CH(CH<sub>3</sub>)<sub>2</sub>  
 4.6296 C<sub>21</sub>H<sub>28</sub>Cl<sub>2</sub>  
 4.7273 C<sub>21</sub>H<sub>29</sub>Br<sub>3</sub>  
 4.7360 (Br•C<sub>6</sub>H<sub>4</sub>Cl)<sub>2</sub>  
 4.7582 C<sub>30</sub>H<sub>50</sub>Cl<sub>2</sub>  
 4.8163 C<sub>56</sub>H<sub>88</sub>Cl<sub>2</sub>  
 4.8716 C<sub>28</sub>H<sub>46</sub>Cl•0.5C<sub>2</sub>H<sub>5</sub>OH  
 5.2479 C<sub>19</sub>H<sub>27</sub>(OH)<sub>2</sub>-CH(CH<sub>3</sub>)CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH(CH<sub>3</sub>)<sub>2</sub>  
 5.2571 Mg<sub>2</sub>(OH)<sub>2</sub>Cl<sub>3</sub>•3H<sub>2</sub>O  
 5.7619 C<sub>19</sub>H<sub>26</sub>(OH)<sub>3</sub>-CH(CH<sub>3</sub>)CH=CHCH(CH<sub>3</sub>)CH(CH<sub>3</sub>)<sub>2</sub>  
 5.9912 C<sub>29</sub>H<sub>44</sub>Cl<sub>7</sub>•0.5H<sub>2</sub>O  
 6.0950 C<sub>14</sub>H<sub>19</sub>N<sub>2</sub>Cl<sub>4</sub>S•Na•3H<sub>2</sub>O  
 6.5010 C<sub>9</sub>H<sub>9</sub>Br<sub>3</sub>•C<sub>10</sub>H<sub>12</sub>Cl<sub>4</sub>  
 7.2464 C<sub>6</sub>H<sub>4</sub>N<sub>4</sub>H<sub>4</sub>•C<sub>8</sub>H<sub>13</sub>N<sub>6</sub>  
 7.2625 C<sub>16</sub>H<sub>20</sub>N<sub>3</sub>Cl<sub>8</sub>Sn•2H<sub>2</sub>O  
 7.6161 C<sub>38</sub>H<sub>18</sub>  
 8.7661 C<sub>7</sub>H<sub>6</sub>BrN<sub>2</sub>  
 8.7974 C<sub>7</sub>H<sub>6</sub>ClN<sub>2</sub>  
 9.1752 C<sub>19</sub>H<sub>28</sub>OH-CH(CH<sub>3</sub>)CH<sub>2</sub>CH<sub>2</sub>Cl(CH<sub>2</sub>)CH(CH<sub>3</sub>)<sub>2</sub>  
 9.2757 C<sub>27</sub>H<sub>44</sub>Cl<sub>4</sub>  
 9.4261 C<sub>19</sub>H<sub>28</sub>OH-CH(CH<sub>3</sub>)CH<sub>2</sub>CH<sub>2</sub>CH(CH<sub>2</sub>H<sub>5</sub>)CH(CH<sub>3</sub>)<sub>2</sub>•H<sub>2</sub>O  
 9.7772 CH<sub>3</sub>•C<sub>6</sub>H<sub>4</sub>•C<sub>19</sub>H<sub>30</sub>-CH(CH<sub>3</sub>)CH<sub>2</sub>CH<sub>2</sub>CH(CH<sub>2</sub>H<sub>5</sub>)CH(CH<sub>3</sub>)<sub>2</sub>  
 9.9733 C<sub>19</sub>H<sub>24</sub>OH-CH(CH<sub>3</sub>)CH=CHCH(CH<sub>3</sub>)CH(CH<sub>3</sub>)<sub>2</sub>•H<sub>2</sub>O  
 11.5217 Cl(C<sub>19</sub>H<sub>28</sub>-CH(CH<sub>3</sub>)CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH(CH<sub>3</sub>)<sub>2</sub>)<sub>2</sub>  
 19.4474 C<sub>19</sub>H<sub>26</sub>(OH)<sub>3</sub>-CH(CH<sub>3</sub>)CH=CHCH(CH<sub>3</sub>)CH(CH<sub>3</sub>)<sub>2</sub>

m

Pm C<sub>s</sub><sup>1</sup> No. 6Inorganic - 1  
Organic - 1

## Inorganic

1.1978 (NH<sub>4</sub>)<sub>2</sub>Cr<sub>4</sub>

## Organic

1.1132 (Cl<sub>3</sub>Co(NH<sub>3</sub>)<sub>4</sub>)<sub>2</sub>S<sub>4</sub>•3H<sub>2</sub>O

m

Pc C<sub>s</sub><sup>2</sup> No. 7Inorganic - 14  
Organic - 31

## Inorganic

0.1876 Ag<sub>3</sub>CuPb<sub>4</sub>Sb<sub>12</sub>S<sub>24</sub>  
 0.6669 S<sub>6</sub>(NH)<sub>2</sub>  
 0.7039 CaAl<sub>2</sub>Si<sub>6</sub>Cl<sub>16</sub>•4H<sub>2</sub>O

0.7936 LiH<sub>3</sub>(SeCl<sub>3</sub>)<sub>2</sub>  
 1.2061 CaB<sub>2</sub>Cl<sub>4</sub>•6H<sub>2</sub>O  
 1.2358 BeLi<sub>2</sub>(SiCl<sub>4</sub>)

Pc C<sub>S</sub><sup>2</sup> No. 7 (continued)

## Inorganic (continued)

1.2755	Na <sub>2</sub> ZnSi $\sigma_4$	1.5417	Al <sub>26</sub> (S $\sigma_4$ ) <sub>6</sub> $\sigma_{33}$ •79H $\sigma_2$
1.3745	HgS $\sigma_4$	1.6279	MnPb <sub>3</sub> H(As $\sigma_3$ ) <sub>3</sub>
1.4523	SmCl <sub>3</sub> •6H $\sigma_2$	2.1203	Pb $\sigma_x$
1.4727	NdCl <sub>3</sub> •6H $\sigma_2$	4.2217	Na <sub>3</sub> HP <sub>2</sub> $\sigma_6$ •9H $\sigma_2$

## Organic

0.4202	$\sigma_2$ NC $\sigma_6$ H $\sigma_4$ C(CN):CHC $\sigma_6$ H $\sigma_4$ N(CH $\sigma_3$ ) <sub>2</sub>	1.7543	K(As(C $\sigma_6$ H $\sigma_4$ $\sigma_2$ ) <sub>2</sub> )
0.6063	C <sub>10</sub> H $\sigma_4$ Br $\sigma_4$	2.0215	(H $\sigma_3$ C) <sub>2</sub> HN•BF $\sigma_3$
0.6245	(C $\sigma_3$ H $\sigma_8$ N) <sub>2</sub> CH $\sigma_2$	2.0319	C <sub>10</sub> H $\sigma_{13}$ ErN $\sigma_2$ $\sigma_8$
0.6753	(CH $\sigma_3$ ) <sub>3</sub> Sn $\sigma_8$ H	2.0691	C $\sigma_6$ H $\sigma_4$ N $\sigma_2$ $\sigma_6$
0.7312	C <sub>23</sub> H $\sigma_{12}$ N $\sigma_2$ $\sigma_2$	2.4353	C $\sigma_6$ H $\sigma_5$ TiCl $\sigma_3$
0.8901	(CH $\sigma_3$ ) <sub>3</sub> NHBr $\sigma_2$	2.8523	LiCl•(CH $\sigma_3$ ) <sub>2</sub> NCH $\sigma_8$
0.9605	C $\sigma_4$ H $\sigma_6$ Cl $\sigma_2$ S $\sigma_2$	2.8907	C $\sigma_5$ H $\sigma_5$ N $\sigma_3$ $\sigma_8$
0.9737	C $\sigma_4$ H $\sigma_6$ BrClS $\sigma_2$	3.3098	C $\sigma_{14}$ H $\sigma_8$ $\sigma_2$
1.2020	C <sub>26</sub> H $\sigma_{18}$ CuN $\sigma_2$ $\sigma_2$	3.4337	C <sub>10</sub> H $\sigma_5$ Cl $\sigma_3$
1.2040	Cu( $\sigma_6$ C $\sigma_6$ H $\sigma_4$ •CH $\sigma_2$ NH•C $\sigma_6$ H $\sigma_4$ ) <sub>2</sub>	3.5228	C <sub>17</sub> H $\sigma_{35}$ C $\sigma_8$ $\sigma_8$ CH=CH $\sigma_2$
1.3321	(C $\sigma_6$ H $\sigma_5$ ) <sub>2</sub> NNC $\sigma_6$ H $\sigma_2$ (N $\sigma_2$ ) <sub>3</sub> •C $\sigma_6$ H $\sigma_6$	3.5242	C <sub>10</sub> H $\sigma_6$ ClN $\sigma_2$
1.3408	(C $\sigma_6$ H $\sigma_5$ ) <sub>2</sub> N $\sigma_2$ C $\sigma_6$ H $\sigma_2$ (N $\sigma_2$ ) <sub>3</sub> •C $\sigma_6$ H $\sigma_6$	3.6036	C <sub>21</sub> H $\sigma_{13}$ N
1.4757	C <sub>10</sub> H $\sigma_6$ $\sigma_2$	3.9095	C $\sigma_6$ H $\sigma_4$ C $\sigma_8$ C $\sigma_6$ H $\sigma_4$ CH $\sigma_2$
1.5595	C <sub>14</sub> H $\sigma_8$ $\sigma_4$	5.6107	C <sub>14</sub> H $\sigma_8$ $\sigma_2$
1.6181	e $\sigma_2$ N•C $\sigma_6$ H $\sigma_4$ •C $\sigma_6$ H $\sigma_4$ N $\sigma_2$	6.2853	(Br[CH $\sigma_2$ ] <sub>14</sub> C $\sigma_8$ $\sigma_8$ ) <sub>2</sub> C $\sigma_3$ H $\sigma_6$ $\sigma_8$
1.7137	C $\sigma_9$ H $\sigma_{12}$ N $\sigma_4$ $\sigma_3$ •C $\sigma_{16}$ H $\sigma_{10}$		

m Cm C<sub>S</sub><sup>3</sup> No. 8 Inorganic - 12  
Organic - 7

## Inorganic

0.5076	Ca(AlSi $\sigma_3$ $\sigma_8$ ) <sub>2</sub> •SH $\sigma_2$ $\sigma_8$	1.1087	KR $\sigma_3$ [( $\sigma_8$ H,F) <sub>2</sub> (Al,Si) $\sigma_4$ $\sigma_{10}$ ]
0.5530	Cd( $\sigma_8$ H,F) $\sigma_2$	1.1491	Al $\sigma_2$ ( $\sigma_8$ H) $\sigma_4$ Si $\sigma_2$ $\sigma_5$ •2H $\sigma_2$ $\sigma_8$
0.5532	Cd( $\sigma_8$ H) $\sigma_2$	1.1517	Al $\sigma_2$ ( $\sigma_8$ H) $\sigma_4$ Si $\sigma_2$ $\sigma_5$ •2H $\sigma_2$ $\sigma_8$
0.8506	Al $\sigma_2$ ( $\sigma_8$ H) $\sigma_4$ Si $\sigma_2$ $\sigma_5$	1.3587	KN $\sigma_2$
0.8600	BaFe $\sigma_2$ Ti $\sigma_8$ (Si $\sigma_2$ $\sigma_7$ )( $\sigma_8$ H) $\sigma_2$	1.5526	Mg $\sigma_3$ H $\sigma_4$ Si $\sigma_2$ $\sigma_6$
1.1031	KMg $\sigma_3$ F $\sigma_2$ AlSi $\sigma_3$ $\sigma_{10}$	4.6789	Ca $\sigma_5$ MgAl $\sigma_2$ $\sigma_{26}$ (Si $\sigma_4$ ) <sub>16</sub>

## Organic

0.0915	C <sub>21</sub> H $\sigma_{42}$ $\sigma_4$	1.7581	(C $\sigma_6$ H $\sigma_{11}$ ) <sub>2</sub> P $\sigma_8$ •SH
0.5578	(NH $\sigma_4$ ) <sub>2</sub> C $\sigma_5$ $\sigma_5$	2.1205	(C $\sigma_{12}$ H $\sigma_8$ N $\sigma_2$ $\sigma_4$ ) <sub>3</sub> •C $\sigma_{12}$ H $\sigma_9$ $\sigma_8$ H
0.5553	(NH $\sigma_4$ ) <sub>2</sub> C $\sigma_5$ $\sigma_5$	5.0886	C $\sigma_7$ H $\sigma_{15}$ N $\sigma_3$ •3HCl
0.8200	H $\sigma_8$ CC $\sigma_2$ C $\sigma_8$ $\sigma_8$		

m Cc C<sub>S</sub><sup>4</sup> No. 9 Inorganic - 31  
Organic - 50

## Inorganic

0.3394	CaZn(Si $\sigma_4$ )•H $\sigma_2$ $\sigma_8$	1.6299	Al $\sigma_2$ ( $\sigma_8$ H) $\sigma_4$ Si $\sigma_2$ $\sigma_5$
0.3943	Li $\sigma_2$ Ge $\sigma_2$ $\sigma_5$	1.7479	Cd $\sigma_4$ GeS $\sigma_5$
0.3970	Li $\sigma_2$ Si $\sigma_2$ $\sigma_5$	1.7745	KCN
0.4159	Na $\sigma_2$ Si $\sigma_2$ $\sigma_5$	1.7770	Sr $\sigma_2$ [B $\sigma_5$ $\sigma_8$ ( $\sigma_8$ H)] <sub>2</sub> •B( $\sigma_8$ H) $\sigma_3$ •H $\sigma_2$ $\sigma_8$
0.5633	CuS $\sigma_4$ •3H $\sigma_2$ $\sigma_8$	1.8323	SrCl $\sigma_2$ •2H $\sigma_2$ $\sigma_8$
0.6766	HCl•3H $\sigma_2$ $\sigma_8$	2.2639	K $\sigma_3$ Mn(CN) $\sigma_5$ N $\sigma_8$ •2H $\sigma_2$ $\sigma_8$
0.9752	CaAl $\sigma_2$ Si $\sigma_3$ $\sigma_{10}$ •3H $\sigma_2$ $\sigma_8$	2.3491	Ca $\sigma_3$ (Si $\sigma_3$ $\sigma_8$ H) $\sigma_2$ •2H $\sigma_2$ $\sigma_8$
1.0312	NaHS $\sigma_4$ •H $\sigma_2$ $\sigma_8$	2.5574	NaTh $\sigma_2$ (P $\sigma_4$ ) <sub>3</sub>
1.1633	VS $\sigma_4$	2.5716	NaU $\sigma_2$ (P $\sigma_4$ ) <sub>3</sub>
1.1728	(NH $\sigma_4$ ) <sub>2</sub> (Mo $\sigma_6$ Cl $\sigma_8$ )Cl $\sigma_6$ •H $\sigma_2$ $\sigma_8$	2.6616	(N $\sigma_2$ ) $\sigma_2$ S $\sigma_3$ $\sigma_{10}$
1.2120	LiNa $\sigma_2$ K(Fe,Mg,Mn) $\sigma_2$ (Ti $\sigma_8$ ) $\sigma_2$ (Si $\sigma_8$ $\sigma_{22}$ )	2.7473	Rb $\sigma_2$ S $\sigma_4$ $\sigma_6$
1.3297	Ce $\sigma_2$ (S $\sigma_4$ ) <sub>3</sub> •5H $\sigma_2$ $\sigma_8$	2.9971	AgSbS $\sigma_2$
1.4974	Al $\sigma_2$ Se $\sigma_3$	3.1307	(Mg,Fe,Al) $\sigma_3$ ( $\sigma_8$ H) $\sigma_2$ (Al,Si) $\sigma_4$ $\sigma_{10}$ •4.32H $\sigma_2$ $\sigma_8$
1.4990	Ge $\sigma_2$ S $\sigma_3$	6.5217	K(Mg,Li) $\sigma_3$ ( $\sigma_8$ H,F) $\sigma_2$ (Al,Si) $\sigma_4$ $\sigma_{10}$
1.6112	Al $\sigma_2$ ( $\sigma_8$ H) $\sigma_4$ Si $\sigma_2$ $\sigma_5$	8.3658	Al $\sigma_4$ ( $\sigma_8$ H) $\sigma_8$ Si $\sigma_4$ $\sigma_{10}$
1.6130	Al $\sigma_2$ ( $\sigma_8$ H) $\sigma_4$ Si $\sigma_2$ $\sigma_5$		

## Organic

0.2723	C(NH $\sigma_2$ ) <sub>3</sub> Br $\sigma_3$	0.8105	(C $\sigma_6$ H $\sigma_5$ ) $\sigma_5$ P
0.4566	(C $\sigma_8$ ) $\sigma_5$ N(CH $\sigma_3$ C $\sigma_8$ C $\sigma_6$ H $\sigma_5$ )	0.8277	(CH $\sigma_3$ ) <sub>3</sub> B $\sigma_3$ N $\sigma_3$ (C $\sigma_6$ H $\sigma_5$ ) <sub>3</sub>
0.4567	(C $\sigma_8$ ) $\sigma_5$ Cr(CH $\sigma_3$ C $\sigma_8$ C $\sigma_6$ H $\sigma_5$ )	0.9071	InC $\sigma_5$ H $\sigma_5$
0.5103	H $\sigma_2$ NC $\sigma_6$ H $\sigma_4$ •CH(C $\sigma_2$ H $\sigma_5$ )•CH(C $\sigma_2$ H $\sigma_5$ )C $\sigma_6$ H $\sigma_4$ NH	0.9167	Tl(C $\sigma_5$ H $\sigma_5$ )
0.8056	(C $\sigma_6$ H $\sigma_5$ ) $\sigma_5$ As	0.9219	IC $\sigma_6$ H $\sigma_4$ N $\sigma_8$



Cc  $C_5^4$  No. 9 (continued)

## Organic (continued)

0.9724	$(C_5H_5)_2NiC_2(C_6H_5)_2$	2.3425	$NH_2CENHCENH_2$
0.9779	$(C_6H_5)_6Co_2[C_2(C_6H_5)_2]$	2.7691	$C_{21}H_{24}F_3N_3S$
1.0247	$Ni(N_2H_3C_6H_5)_3 \cdot N_2H_5 \cdot H_2O$	2.9719	$C_6H_5NH_3Cl$
1.0279	$Ni(N_2H_3C_6H_5)_3 \cdot N_2H_5 \cdot H_2O$	3.0364	$[(CH_3)_2PBH_2]_4$
1.0473	$C_4F_4[As(CH_3)_2]_2[Fe(C_6H_5)_3]_2$	3.0525	$C_{12}H_{10}$
1.0831	$C_5H_9S_5SNCu$	3.2044	$C_{16}H_{18}N_2O_3$
1.1124	$Fe(C_6H_5)_3C_6H_6Fe(C_6H_5)_3$	3.3241	$S(CH_2 \cdot CH_2 \cdot C_6H_5)_2$
1.1526	$(C_{12}H_8N_2)_2Cl_2CoCl \cdot 3H_2O$	3.9206	$LiOOC_2Cl_3 \cdot H_2O$
1.2553	$Pb(C_5H_{10}NS_2)_2$	4.8326	$Hg(SC_2H_5)_2$
1.3064	$C_{12}H_4N_7O_{12}CS$	4.8871	$Hg(SC_2H_5)_2$
1.3919	$(C_{12}H_8N_2O_4)_4 \cdot (C_{12}H_{12}N_2)$	4.9863	$Hg(SC_3H_7)_2$
1.4061	$N(C_6H_5)_3$	5.1552	$C_6H_{11}N_3O_4 \cdot 0.5H_2O$
1.4095	$Au(C_{18}H_{12}N_2)Cl_3$	5.2551	$C_{10}H_4Br_5NO$
1.5353	$N_3B_3(CH_3)_3$	5.2968	$C_{10}H_7OH$
1.6984	$CH_3NC_{18}H_{16} \cdot HN_3$	6.5655	$Hg(SC_5H_{11})_2$
1.7745	KCN	6.8149	$C_{17}H_{35}C_6O_2H_5$
1.8784	$C_6H_9O_3P_6$	7.6130	$Hg(SC_6H_{13})_2$
1.8943	$(CH_2O)_2P_6O_2CH_3$	8.1736	$Hg(SC_7H_{15})_2$
2.2639	$K_3Mn(CN)_5 \cdot N_2O \cdot 2H_2O$	9.0182	$C_{12}H_{10}BN_2O$
2.3087	$[(C_2H_5)_3P]_2 \cdot Ni(N_3)_2$	10.0080	$C_{14}H_8N_4KAu$

 $\frac{2}{m}$ P2/m  $C_{2h}^1$  No. 10Inorganic - 26  
Organic - 13

## Inorganic

0.3014	$Ga_9S_8Cl_{11}$	1.5870	$Mg_{z/2}(Mg, Fe, Mn)_{3-x/2-3y/2}(Al, Fe)_y(Si_{2-z}Al_z)_{5-x}(OH)_{4+x}$
0.3125	$Ga_9S_8Br_{11}$	2.0857	$Ca_4MgH_6(BO_3)_4(CO_3)_2$
0.6836	$CaC_2O_4 \cdot H_2O$	3.3787	$Na_2V_6O_{16} \cdot 3H_2O$
0.7215	$Al_2(P_6O_4)(V_6O_4) \cdot 8H_2O$	3.8212	$IrU_2$
0.7651	$Al_2(P_6O_4)(V_6O_4) \cdot 6H_2O$	3.8357	$RhU_2$
0.8358	$Al_2Fe(S_6O_4)_4 \cdot 22H_2O$	3.9204	$RuU_2$
0.8595	$Al_2Mg(S_6O_4)_4 \cdot 22H_2O$	4.0078	$OsU_2$
0.8790	$As_4CoFe$	4.0987	$TcU_2$
1.0622	$Mo_6O_3 \cdot 2H_2O$	4.4617	$Pb_2Bi_4S_5Se_3$
1.0766	$H_2W_6O_{24} \cdot 2H_2O$	4.6489	$Pb_5Sb_6S_{17}$
1.0912	$Mo_6O_3 \cdot 2H_2O$	4.6834	$W_{18}O_{49}$
1.1902	$Hg_4H_2O_4Cl_2$	6.1905	$W_{20}O_{58}$
1.5791	$(Mg, Fe, Mn)_{3-[(x+3y)/2]}(Al, Fe)_ySi_2O_{5-x}(OH)_{4+x}$	7.7940	$W_{62}O_{96}$

## Organic

0.3501	$CH_3H_4C_6 \cdot C_6H_3 \cdot CH_3NO_2$	1.1741	$C(CH_2I)_4$
0.6581	$C_4H_3O \cdot CH : N \cdot NH \cdot C_6H_3(NO_2)_2$	1.2941	$C_3H_4N_2$
0.6836	$Ca(C_2O_4) \cdot H_2O$	1.3765	$(CH_3)_2H_3C_6 \cdot C_6H_3CH_3NO_2$
0.7128	$[Cu(CH_2)_4NH(NH_2)_2Cl]Cl \cdot 0.5H_2O$	1.4332	$C_{14}H_8O_2$
0.9982	$C_5H_4N \cdot CH_3$	1.5107	$YNH_4(C_2O_4)_2 \cdot H_2O$
1.0991	$C(CH_2Cl)_4$	2.2812	$NH_2CH_2C_6H_4Ag$
1.1382	$C(CH_2Br)_4$		

 $\frac{2}{m}$ P2<sub>1</sub>/m  $C_{2h}^2$  No. 11Inorganic - 123  
Organic - 77

## Inorganic

0.2803	$Pb_27As_{14}S_{48}$	0.8589	$AgNC_6$
0.2807	$Pb_{13}As_7S_{23}$	0.8667	$Li_4Si_6O_4$
0.2813	$Pb_5(Sb, As)_2S_8$	0.8810	$Fe(OH)SO_4 \cdot 2H_2O$
0.2914	$AlNa(S_6O_4)_2 \cdot 6H_2O$	0.8889	$Li_4Ge_6O_4$
0.4423	$(Sr, Ba, Ca)(Al_2Si_6O_{16}) \cdot 5H_2O$	0.8933	$FeP_6O_4 \cdot 2H_2O$
0.4877	$Pb_2(U_6O_2)_3(OH)_4(P_6O_4)_2 \cdot 3H_2O$	0.8957	$Fe_2(OH)_3Br$
0.5459	$(NSCl)_3$	0.9117	$KV_3O_8$
0.6438	$KCuBr_3$	0.9192	$Ni_2(OH)_3Br$
0.7090	$CoSO_4$	0.9213	$Co_2(OH)_3Br$
0.7837	$N_2H_4$	0.9329	$Cu_2(OH)_3Cl$
0.8009	$K_3(U_6O_2)_2F_7 \cdot 2H_2O$	0.9597	$CsV_3O_8$
0.8147	$(Mg, Mn, Zn)_8(OH)_{14}S_6O_4 \cdot 4H_2O$	0.9615	$Mn_2(OH)_3I$
0.8377	$MnCl_2 \cdot 2H_2O$	0.9716	$W_6O_{29}$
0.8513	$XeF_6$	0.9771	$Fe_2(OH)_3I$
0.8533	$CoCl_2 \cdot 2H_2O$	0.9865	$Cu_2(OH)_3Br$

P2<sub>1</sub>/m C<sub>2h</sub><sup>2</sup> No. 11 (continued)

## Inorganic (continued)

1.0000	AlLa <sub>3</sub>	1.3660	CaK <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •H <sub>2</sub> O
1.0000	AlY <sub>3</sub>	1.4323	K <sub>2</sub> [Pt(NH <sub>2</sub> ) <sub>3</sub> Cl <sub>3</sub> ]
1.0000	NH <sub>4</sub> I <sub>3</sub>	1.4481	(Mn, Fe)Pb <sub>2</sub> (V <sub>6</sub> ) <sub>2</sub> •H <sub>2</sub> O
1.0000	BaCe <sub>3</sub>	1.5000	CuPb <sub>2</sub> (P <sub>4</sub> )(SO <sub>4</sub> )(OH)
1.0000	BaPr <sub>3</sub>	1.5124	(Sr, Ba, Na) <sub>2</sub> AlF <sub>5</sub> (CO <sub>3</sub> )
1.0000	BaTh <sub>3</sub>	1.5434	RbNH <sub>2</sub>
1.0000	CdCe <sub>3</sub>	1.5565	InOHSO <sub>4</sub> •2H <sub>2</sub> O
1.0000	CdCaCl <sub>3</sub>	1.5940	KNH <sub>2</sub>
1.0000	CdTh <sub>3</sub>	1.6147	Ba(Fe, Mg)(Fe, Mn)Ti(Si <sub>2</sub> O <sub>7</sub> )(OH, Cl)(OH, Cl)
1.0000	CdSn <sub>3</sub>	1.6301	YOH
1.0000	CdTl <sub>3</sub>	1.6374	HoOH
1.0000	CaCe <sub>3</sub>	1.6397	YbOH
1.0000	CaTh <sub>3</sub>	1.6409	ErOH
1.0000	CaSn <sub>3</sub>	1.7133	CuPb(OH) <sub>2</sub> SO <sub>4</sub>
1.0000	CaTi <sub>3</sub>	1.7434	LiAlSi <sub>2</sub> O <sub>6</sub> •H <sub>2</sub> O
1.0000	CePb <sub>3</sub>	1.7446	KFe(SO <sub>4</sub> ) <sub>2</sub> •H <sub>2</sub> O
1.0000	CaZr <sub>3</sub>	1.7526	Ba(NH <sub>2</sub> NHSO <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> O
1.0000	CeMg <sub>3</sub>	1.7774	(Ca, X) <sub>x</sub> (Fe, Al)Si <sub>3</sub> O <sub>12</sub>
1.0000	CeSr <sub>3</sub>	1.7887	Ca <sub>2</sub> (Al, Fe, Mn) <sub>3</sub> Si <sub>3</sub> O <sub>12</sub> (OH)
1.0000	CsI <sub>3</sub>	1.7951	Ca <sub>2</sub> (Al, Fe, Mn) <sub>3</sub> Si <sub>3</sub> O <sub>12</sub> (OH)
1.0000	HfSr <sub>3</sub>	1.8036	Al <sub>2</sub> (Al, Fe)OHCa <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>
1.0000	PbTh <sub>3</sub>	1.8045	Pb <sub>3</sub> CuO <sub>2</sub> (OH) <sub>2</sub> Cl <sub>2</sub>
1.0000	KMgF <sub>3</sub>	1.8117	Al <sub>2</sub> (Al, Fe)Ca <sub>2</sub> OH(SiO <sub>4</sub> ) <sub>3</sub>
1.0000	KNiF <sub>3</sub>	1.8169	Ca <sub>2</sub> Al <sub>3</sub> (OH)(SiO <sub>4</sub> ) <sub>3</sub>
1.0000	KI <sub>3</sub>	1.8206	Al <sub>2</sub> Ca <sub>2</sub> FeOH(OH)(Si <sub>2</sub> O <sub>7</sub> )(SiO <sub>4</sub> )
1.0000	KZnF <sub>3</sub>	1.8232	Ca <sub>2</sub> Al <sub>3</sub> (OH)(SiO <sub>4</sub> ) <sub>3</sub>
1.0000	RbI <sub>3</sub>	1.8232	Y(OH) <sub>2</sub> Cl
1.0000	NaTa <sub>3</sub>	1.8428	Mg <sub>3</sub> Mn <sub>3</sub> B <sub>2</sub> O <sub>10</sub>
1.0000	SrTh <sub>3</sub>	1.9847	Ni <sub>3</sub> Te <sub>2</sub>
1.0000	SnSr <sub>3</sub>	2.0730	Rb <sub>x</sub> (UO <sub>2</sub> ) <sub>x</sub> Cl <sub>x</sub>
1.0000	SrZr <sub>3</sub>	2.0905	K <sub>x</sub> (UO <sub>2</sub> ) <sub>x</sub> Cl <sub>x</sub>
1.0023	Co <sub>2</sub> (OH) <sub>3</sub> I	2.1209	Cs <sub>0.9</sub> (UO <sub>2</sub> ) <sub>0.9</sub> Cl <sub>0.9</sub>
1.0028	CaSn <sub>3</sub>	2.1310	Ca <sub>3</sub> Pb(ZnSiO <sub>4</sub> ) <sub>4</sub>
1.0049	Ni <sub>2</sub> (OH) <sub>3</sub> I	2.2745	Pu
1.0655	Cu <sub>2</sub> (OH) <sub>3</sub> I	2.3092	K <sub>x</sub> (UO <sub>2</sub> ) <sub>x</sub> Br <sub>x</sub>
1.1036	(NH <sub>4</sub> ) <sub>4</sub> [Ir(SO <sub>3</sub> ) <sub>2</sub> Cl <sub>3</sub> ]•4H <sub>2</sub> O	2.4014	Na <sub>2</sub> Ti <sub>3</sub> O <sub>7</sub>
1.1132	Mo(OH) <sub>3</sub> PO <sub>4</sub>	2.5066	ZrSe <sub>3</sub>
1.1398	Cu <sub>2</sub> (OH) <sub>3</sub> N <sub>3</sub>	2.7260	Pb <sub>4</sub> As <sub>6</sub> S <sub>13</sub>
1.1942	PbSe <sub>3</sub>	2.7370	Pb <sub>3</sub> As <sub>4</sub> S <sub>9</sub>
1.2000	Na <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> •2H <sub>2</sub> O	2.9763	TaSe <sub>3</sub>
1.2197	K <sub>2</sub> S <sub>2</sub> O <sub>5</sub>	3.2031	[Pb <sub>6</sub> (Ag, Cu) <sub>2</sub> As <sub>4</sub> S <sub>13</sub> ]
1.2241	K <sub>2</sub> S <sub>2</sub> O <sub>5</sub>	3.2889	Li <sub>1+x</sub> V <sub>3</sub> O <sub>8</sub>
1.2558	Th(OH) <sub>2</sub> Cr <sub>6</sub> •H <sub>2</sub> O	3.4111	(Na, Ca) <sub>2</sub> V <sub>6</sub> O <sub>16</sub>
1.2618	KCl <sub>3</sub>	3.4246	(Na, Ca) <sub>2</sub> V <sub>6</sub> O <sub>16</sub> •2H <sub>2</sub> O
1.3218	Mg <sub>3</sub> Si <sub>2</sub> O <sub>7</sub> •2H <sub>2</sub> O	3.9954	MoTe <sub>2</sub>
1.3348	Na <sub>3</sub> Mg(PO <sub>4</sub> )(CO <sub>3</sub> )	14.1020	Pb <sub>2</sub> (Cu, Ag) <sub>3</sub> Bi <sub>5</sub> S <sub>11</sub>
1.3394	CaK <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •H <sub>2</sub> O		

## Organic

0.0915	C <sub>21</sub> H <sub>42</sub> O <sub>4</sub>	0.7028	C <sub>8</sub> H <sub>8</sub> Mo(CO) <sub>3</sub>
0.3085	C <sub>11</sub> H <sub>9</sub> N <sub>2</sub> O <sub>3</sub> Cl	0.7255	Co <sub>2</sub> (CO) <sub>8</sub>
0.3115	C <sub>4</sub> H <sub>8</sub> S <sub>2</sub> •CRI <sub>3</sub>	0.7330	[C <sub>5</sub> H <sub>5</sub> Rh(CO)] <sub>3</sub>
0.3697	(C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> SF•2.3H <sub>2</sub> O	0.7519	C <sub>4</sub> Cl <sub>8</sub>
0.4174	C <sub>10</sub> H <sub>7</sub> Cl	0.7545	Cu(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>2</sub> •2H <sub>2</sub> O•C <sub>6</sub> H <sub>5</sub> (NO <sub>2</sub> ) <sub>3</sub> O
0.4207	C <sub>4</sub> H <sub>2</sub> O(CO <sub>2</sub> H) <sub>2</sub>	0.7757	(C <sub>9</sub> H <sub>5</sub> O <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub>
0.4248	Ni(NH <sub>2</sub> •CS•NH•NH <sub>2</sub> ) <sub>2</sub> SO <sub>4</sub> •3H <sub>2</sub> O	0.7981	CH <sub>5</sub> N•BF <sub>3</sub>
0.4286	C <sub>8</sub> H <sub>12</sub> S <sub>2</sub> Hg <sub>2</sub> Cl <sub>4</sub>	0.8407	(CH <sub>3</sub> ) <sub>3</sub> N•HBr
0.4732	C <sub>5</sub> H <sub>9</sub> N <sub>3</sub>	0.8524	C <sub>6</sub> H <sub>2</sub> CNBr <sub>3</sub>
0.5122	C <sub>8</sub> H <sub>16</sub> N <sub>10</sub> O <sub>9</sub>	0.8551	(CH <sub>3</sub> ) <sub>3</sub> N•HI
0.5131	C <sub>17</sub> H <sub>10</sub> O <sub>4</sub> N <sub>2</sub>	0.8588	C <sub>8</sub> H <sub>10</sub> O
0.5727	C <sub>5</sub> H <sub>5</sub> N•C(CN) <sub>2</sub>	0.8589	AgNC <sub>6</sub>
0.5868	Re <sub>2</sub> Cl <sub>5</sub> (C <sub>4</sub> H <sub>10</sub> S <sub>2</sub> ) <sub>2</sub>	0.8743	C <sub>5</sub> H <sub>8</sub> SO <sub>2</sub>
0.5935	C <sub>6</sub> H <sub>6</sub> Cr(CO) <sub>3</sub>	0.8962	Pt(C <sub>2</sub> H <sub>4</sub> )[NH(CH <sub>3</sub> ) <sub>2</sub> ]Cl <sub>2</sub>
0.5967	C <sub>7</sub> H <sub>6</sub> C(CN) <sub>2</sub>	0.8993	(CH <sub>3</sub> ) <sub>3</sub> SI
0.5971	C <sub>3</sub> N <sub>3</sub> (N[CH <sub>3</sub> ]) <sub>2</sub> •C <sub>6</sub> H <sub>3</sub> (NO <sub>2</sub> ) <sub>3</sub>	0.9397	C <sub>5</sub> H <sub>5</sub> N•HCl
0.5987	C <sub>6</sub> H <sub>6</sub> Cr(CO) <sub>3</sub>	0.9460	C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>
0.6075	AgNO <sub>3</sub> •CO(NH <sub>2</sub> ) <sub>2</sub>	1.0123	CH <sub>3</sub> CO•SbF <sub>6</sub>
0.6163	C <sub>4</sub> H <sub>4</sub> SCr(CO) <sub>3</sub>	1.0469	CH <sub>3</sub> OH
0.6410	TiCl <sub>3</sub> (C <sub>5</sub> H <sub>5</sub> )	1.0590	CN•C•CH
0.6562	(NH <sub>3</sub> ) <sub>2</sub> PdC <sub>2</sub> O <sub>4</sub>	1.0643	B <sub>9</sub> H <sub>13</sub> (CH <sub>3</sub> CN)
0.6616	C <sub>11</sub> H <sub>8</sub> O <sub>2</sub>	1.1375	C <sub>10</sub> H <sub>20</sub> (C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> SO <sub>2</sub>
0.6768	C <sub>6</sub> H <sub>3</sub> NH <sub>2</sub> (NO <sub>2</sub> ) <sub>2</sub>	1.1384	I•C•C•CN
0.6821	HMn <sub>3</sub> (CO) <sub>10</sub> (BH <sub>3</sub> ) <sub>2</sub>	1.1462	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> (C <sub>2</sub> H <sub>2</sub> ) <sub>2</sub>

P2<sub>1</sub>/m C<sub>2h</sub><sup>2</sup> No. 11 (continued)

## Organic (continued)

1.1623	Pm <sub>2</sub> (C <sub>2</sub> θ <sub>4</sub> ) <sub>3</sub> •10H <sub>2</sub> θ	1.3748	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> •HCl
1.1630	Sm <sub>2</sub> (C <sub>2</sub> θ <sub>4</sub> ) <sub>3</sub> •10H <sub>2</sub> θ	1.4067	ICH <sub>3</sub> NC <sub>5</sub> H <sub>4</sub> CH•NθH
1.1658	Nd <sub>2</sub> (C <sub>2</sub> θ <sub>4</sub> ) <sub>3</sub> •10H <sub>2</sub> θ	1.4486	C <sub>14</sub> H <sub>8</sub> θ <sub>2</sub>
1.1712	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub>	1.4517	C <sub>14</sub> H <sub>13</sub> Nθ <sub>2</sub>
1.1979	Pu <sub>2</sub> (C <sub>2</sub> θ <sub>4</sub> ) <sub>3</sub> •10H <sub>2</sub> θ	1.6234	Cu(C <sub>12</sub> H <sub>18</sub> N <sub>2</sub> θ <sub>2</sub> )•CH <sub>3</sub> NH <sub>3</sub> Clθ <sub>4</sub>
1.2571	C <sub>6</sub> H <sub>5</sub> Nθ <sub>3</sub>	1.6837	C <sub>6</sub> H <sub>4</sub> Nθ•CH <sub>3</sub>
1.2662	BaTe(S <sub>2</sub> θ <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> θ•(CH <sub>2</sub> ) <sub>4</sub> θ	1.7206	Fe(C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> θ <sub>2</sub> )Cl
1.2680	BaSe(S <sub>2</sub> θ <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> θ•(CH <sub>3</sub> ) <sub>2</sub> Cθ	1.7597	Cu(NH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> Cθθ) <sub>2</sub> •2H <sub>2</sub> θ
1.2694	BaSe(S <sub>2</sub> θ <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> θ•(CH <sub>2</sub> ) <sub>4</sub> θ	1.9149	C <sub>20</sub> H <sub>13</sub> N
1.2722	BaS(S <sub>2</sub> θ <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> θ•(CH <sub>3</sub> ) <sub>2</sub> Cθ	1.9520	C <sub>11</sub> H <sub>17</sub> Nθ
1.2794	BaS(S <sub>2</sub> θ <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> θ•(CH <sub>2</sub> ) <sub>4</sub> θ	1.9592	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> θ <sub>2</sub> -C <sub>6</sub> H <sub>7</sub> N <sub>5</sub>
1.2805	AlCl <sub>3</sub> •C <sub>6</sub> H <sub>5</sub> CθCl	2.0947	C <sub>6</sub> H <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> (Nθ <sub>2</sub> ) <sub>2</sub>
1.3148	C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>	2.5166	HClθ <sub>4</sub> •2[(CH <sub>3</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>2</sub> Cθθ]
1.3348	Na <sub>3</sub> Mg(Pθ <sub>4</sub> )(Cθ <sub>3</sub> )	2.7101	C <sub>6</sub> H <sub>4</sub> •C <sub>2</sub> H <sub>5</sub> θ•Cθ•HgBr
1.3354	C <sub>2</sub> H <sub>5</sub> NH <sub>3</sub> •Br		

2	C2/m	C <sub>3h</sub> <sup>3</sup>	No. 12	Inorganic - 310
m				Organic - 47

## Inorganic

0.3953	(Mn, Mg, Fe) <sub>14</sub> (Al, Fe) <sub>4</sub> Sb <sub>2</sub> Si <sub>2</sub> θ <sub>29</sub>	0.5781	HoCl <sub>3</sub>
0.4736	(Fe, Mg) <sub>4</sub> Al <sub>18</sub> Si <sub>8</sub> θ <sub>46</sub> (θH) <sub>2</sub>	0.5793	LuCl <sub>3</sub>
0.4963	Mg <sub>8</sub> H <sub>6</sub> Si <sub>12</sub> θ <sub>30</sub> (θH) <sub>10</sub> +aq.	0.5796	YCl <sub>3</sub>
0.5196	(Mg, Fe) <sub>7</sub> (θH) <sub>2</sub> (Si <sub>4</sub> θ <sub>11</sub> ) <sub>2</sub>	0.5854	RhCl <sub>3</sub>
0.5225	(Fe, Mg) <sub>7</sub> Si <sub>8</sub> (θ, θH) <sub>24</sub>	0.5924	CrCl <sub>3</sub>
0.5228	(Mg, Fe, Mn, Ca) <sub>7</sub> (Si, Al) <sub>8</sub> θ <sub>22</sub> (θH) <sub>2</sub>	0.6027	NbS <sub>2</sub> Cl <sub>2</sub>
0.5242	(Fe, Mg, Mn) <sub>7</sub> (Si, Al) <sub>8</sub> θ <sub>22</sub> (θH) <sub>2</sub>	0.6027	Al <sub>2</sub> Cl <sub>6</sub>
0.5246	(Mg, Fe) <sub>7</sub> (θH) <sub>2</sub> (Si <sub>4</sub> θ <sub>11</sub> ) <sub>2</sub>	0.6043	AlBrCl <sub>2</sub>
0.5251	Fe <sub>7</sub> (θH) <sub>2</sub> (Si <sub>4</sub> θ <sub>11</sub> ) <sub>2</sub>	0.6179	Na(Ca, Na) <sub>2</sub> (Al <sub>5</sub> Si <sub>13</sub> θ <sub>36</sub> )•17H <sub>2</sub> θ
0.5254	(Fe, Mg, Mn) <sub>7</sub> (θH) <sub>2</sub> (Si <sub>4</sub> θ <sub>11</sub> ) <sub>2</sub>	0.6227	Ca <sub>2</sub> NaAl <sub>5</sub> Si <sub>13</sub> θ <sub>36</sub> •14H <sub>2</sub> θ
0.5266	(Mg, Mn, Ca, Fe) <sub>7</sub> (Si <sub>4</sub> θ <sub>11</sub> ) <sub>2</sub> (θH) <sub>2</sub>	0.6263	(Uθ <sub>2</sub> ) <sub>3</sub> (θH) <sub>2</sub> (Sθ <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> θ
0.5362	Na <sub>2</sub> (Mg, Fe) <sub>3</sub> Al <sub>2</sub> Si <sub>8</sub> θ <sub>22</sub> (θH) <sub>2</sub>	0.6431	(K, Na)AlSi <sub>3</sub> θ <sub>8</sub>
0.5385	(Na, Ca, K) <sub>3</sub> (Fe, Mn) <sub>5</sub> (Si, Al) <sub>8</sub> θ <sub>22</sub> (θH) <sub>2</sub>	0.6438	(K, Na)AlSi <sub>3</sub> θ <sub>8</sub>
0.5385	Na <sub>2</sub> Fe <sub>3</sub> Fe <sub>2</sub> Si <sub>8</sub> θ <sub>22</sub> (θH) <sub>2</sub>	0.6457	KAlSi <sub>3</sub> θ <sub>8</sub>
0.5390	(Na, Ca, K) <sub>2</sub> (Mg, Fe)(Fe, Al) <sub>2</sub> Si <sub>8</sub> θ <sub>22</sub> (θH) <sub>2</sub>	0.6457	(K, Na)AlSi <sub>3</sub> θ <sub>8</sub>
0.5403	(Ca, Na, K) <sub>3</sub> (Mg, Fe, Al) <sub>6</sub> [(Si, Al)θ <sub>3</sub> ] <sub>8</sub>	0.6465	KAlSi <sub>3</sub> θ <sub>8</sub>
0.5415	(Na, Ca, K) <sub>3</sub> (Fe, Mg) <sub>5</sub> (Si, Al) <sub>8</sub> θ <sub>23</sub> θH	0.6471	KAlSi <sub>3</sub> θ <sub>8</sub>
0.5415	Fe <sub>2</sub> Mg <sub>3</sub> Na <sub>2</sub> Si <sub>8</sub> θ <sub>22</sub> (θH) <sub>2</sub>	0.6485	KAlSi <sub>3</sub> θ <sub>8</sub>
0.5419	Na <sub>2</sub> Mg <sub>3</sub> Al <sub>2</sub> Si <sub>8</sub> θ <sub>22</sub> (θH) <sub>2</sub>	0.6488	KAlSi <sub>3</sub> θ <sub>8</sub>
0.5421	(Na, Ca, K) <sub>3</sub> (Mg, Fe, Ti) <sub>5</sub> (Si, Al) <sub>8</sub> (θ, θH) <sub>24</sub>	0.6494	MoCl <sub>3</sub>
0.5432	Ca <sub>2</sub> Mg <sub>5</sub> F <sub>2</sub> (Si <sub>4</sub> θ <sub>11</sub> ) <sub>2</sub>	0.6496	BaAl <sub>2</sub> Si <sub>2</sub> θ <sub>8</sub>
0.5433	Fe <sub>2</sub> Mg <sub>3</sub> Na <sub>2</sub> (θH) <sub>2</sub> Si <sub>8</sub> θ <sub>22</sub>	0.6504	(Ba, K)Al <sub>2</sub> Si <sub>2</sub> θ <sub>8</sub>
0.5433	[H <sub>2</sub> (Ca, Na, K) <sub>2</sub> (Mg, Fe, Na) <sub>5</sub> (Siθ <sub>3</sub> ) <sub>8</sub> ]	0.6517	FeKSi <sub>3</sub> θ <sub>8</sub>
0.5440	Na <sub>2</sub> Fe <sub>5</sub> Si <sub>8</sub> θ <sub>22</sub> (θH, F) <sub>2</sub>	0.6538	KAlSi <sub>3</sub> θ <sub>8</sub>
0.5442	AlCa <sub>2</sub> Mg <sub>4</sub> Na(θH) <sub>2</sub> Si <sub>6</sub> Al <sub>2</sub> θ <sub>22</sub>	0.6636	Ca <sub>7</sub> (Siθ <sub>3</sub> ) <sub>6</sub> (Cθ <sub>3</sub> )•2H <sub>2</sub> θ
0.5445	Ca <sub>2</sub> Mg <sub>3</sub> •5Fe <sub>1</sub> •5(θH) <sub>2</sub> AlSi <sub>7</sub> θ <sub>22</sub>	0.6654	U
0.5447	NaCa <sub>2</sub> (Fe, Mg) <sub>4</sub> FeAl <sub>2</sub> Si <sub>6</sub> θ <sub>22</sub> (θH) <sub>2</sub>	0.6667	NbF <sub>5</sub>
0.5448	Ca <sub>2</sub> (Mg, Fe) <sub>5</sub> Si <sub>8</sub> θ <sub>22</sub> (θH) <sub>2</sub>	0.6671	TaF <sub>5</sub>
0.5448	(K, Na) <sub>0.5</sub> (Ca, Na, K) <sub>2</sub> (Mg, Fe) <sub>3</sub> (Fe, Al, Ti) <sub>2</sub>	0.6758	MoF <sub>5</sub>
	Al <sub>2</sub> Si <sub>6</sub> θ <sub>25</sub>	0.6805	SrNi(CN) <sub>4</sub> •5H <sub>2</sub> θ
0.5451	Ca <sub>2</sub> Mg <sub>5</sub> (θH) <sub>2</sub> Si <sub>8</sub> θ <sub>22</sub>	0.6845	SrPt(CN) <sub>4</sub> •5H <sub>2</sub> θ
0.5451	NaCa <sub>2</sub> (Fe, Mg) <sub>4</sub> (Fe, Al)Al <sub>2</sub> Si <sub>6</sub> θ <sub>22</sub> (θH) <sub>2</sub>	0.6860	SrPd(CN) <sub>4</sub> •5H <sub>2</sub> θ
0.5461	BCa <sub>2</sub> Mg <sub>5</sub> NaF <sub>2</sub> Si <sub>7</sub> θ <sub>22</sub>	0.7149	GePt <sub>3</sub>
0.5465	[Ca <sub>2</sub> Mg <sub>5</sub> Si <sub>8</sub> θ <sub>22</sub> (θH) <sub>2</sub> ]	0.7161	Pt <sub>3</sub> Si
0.5465	Na <sub>3</sub> (Fe, Mn) <sub>5</sub> Si <sub>8</sub> θ <sub>22</sub> (θH) <sub>2</sub>	0.7222	Mg <sub>5</sub> (θH) <sub>2</sub> Si <sub>8</sub> θ <sub>20</sub> (θH <sub>2</sub> ) <sub>4</sub> •4H <sub>2</sub> θ
0.5466	(Na, K, Ca) <sub>3</sub> (Mg, Fe, Fe, Ti, Al) <sub>5</sub> (Si, Al) <sub>8</sub> (θ, θH) <sub>24</sub>	0.7437	Fe <sub>3</sub> (Pθ <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> θ
0.5469	AlCa <sub>2</sub> Mg <sub>5</sub> NaF <sub>2</sub> Si <sub>7</sub> θ <sub>22</sub>	0.7451	Fe <sub>3</sub> (Pθ <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> θ
0.5469	H <sub>2</sub> (Ca, Na, K) <sub>2-3</sub> (Mg, Fe, Al) <sub>5</sub> [(Si, Al)θ <sub>3</sub> ] <sub>8</sub>	0.7528	Na <sub>2</sub> [Ru(Nθ <sub>2</sub> ) <sub>4</sub> (Nθ)(θH)]•2H <sub>2</sub> θ
0.5470	(Na, K, Ca, Fe, Fe) <sub>7</sub> (θH) <sub>2</sub> (Si, Al) <sub>8</sub> θ <sub>22</sub>	0.7538	Co <sub>3</sub> (Asθ <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> θ
0.5470	(Ca, Na) <sub>2</sub> Mg <sub>5</sub> NaF <sub>2</sub> (Si <sub>4</sub> θ <sub>11</sub> ) <sub>2</sub>	0.7540	Ni <sub>3</sub> (Asθ <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> θ
0.5471	(Ca, Na, K) <sub>2</sub> •64(Si, Al) <sub>8</sub> Fe <sub>1</sub> •42(Fe, Mn, Mg, Ti) <sub>3</sub> •54(θH) <sub>2</sub> •15θ <sub>22</sub>	0.7545	Mg <sub>3</sub> (Asθ <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> θ
		0.7573	Zn <sub>3</sub> (Asθ <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> θ
0.5472	Na <sub>3</sub> (Mg, Fe) <sub>4</sub> (Fe, Al)Si <sub>8</sub> θ <sub>22</sub> (θH, F) <sub>2</sub>	0.7574	Fe <sub>3</sub> (Asθ <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> θ
0.5490	Na <sub>2</sub> Fe <sub>2</sub> (Fe, Mg) <sub>3</sub> Si <sub>8</sub> θ <sub>22</sub> (θH) <sub>2</sub>	0.7646	Sc <sub>2</sub> Si <sub>2</sub> θ <sub>7</sub>
0.5527	(Na, K, Ca) <sub>3</sub> (Fe, Mn, Mg, Ti, Al) <sub>5</sub> (Si <sub>8</sub> θ <sub>22</sub> )(θH, F) <sub>2</sub>	0.7727	Mn <sub>2</sub> P <sub>2</sub> θ <sub>7</sub>
0.5754	TmCl <sub>3</sub>	0.7740	Mg <sub>2</sub> As <sub>2</sub> θ <sub>7</sub>
0.5768	ErCl <sub>3</sub>	0.7838	Mg <sub>2</sub> P <sub>2</sub> θ <sub>7</sub>
0.5772	TlCl <sub>3</sub>	0.7964	Zn <sub>2</sub> P <sub>2</sub> θ <sub>7</sub>
0.5773	DyCl <sub>3</sub>	0.8402	LiθH•H <sub>2</sub> θ
0.5775	InCl <sub>3</sub>	0.8419	MnCl <sub>2</sub> •2H <sub>2</sub> θ
0.5776	IrCl <sub>3</sub>	0.8510	CoCl <sub>2</sub> •2H <sub>2</sub> θ
0.5777	YbCl <sub>3</sub>	0.8562	CoCl <sub>2</sub> •2H <sub>2</sub> θ

C2/m  $C_{2h}^3$  No. 12 (continued)

## Inorganic (continued)

0.8597	$KNaPt(CN)_4 \cdot 3H_2O$	1.5734	$RbCr_3O_8$
0.8604	$FeCl_2 \cdot 2H_2O$	1.6104	$Li_2SnO_3$
0.8676	$CuF_2 \cdot 2H_2O$	1.6341	$(Au, Ag)_2Te_2$
0.8873	Pu	1.6577	$Na_2TbO_3$
0.8904	$Al_2CaSi_7O_{18} \cdot 6H_2O$	1.6698	$Li_2MnO_3$
0.9719	$MoCl_5$	1.6717	$Na_2PbO_3$
1.0037	$Cu(NH_3)_2Br_2$	1.6833	$Na_2Ni(CN)_4 \cdot 3H_2O$
1.0189	$Nb_2Cl_{10}$	1.7026	$Na_2HfO_3$
1.0822	$(Ca, Mg, Al)_4(OH)_2(Si, Al)_4O_{10}$	1.7051	$Na_2SnO_3$
1.0893	$CoMoO_4$	1.7281	$K_2(Mg, Al)_9(OH)_6[(Si, Al)_4O_{10}]_3$
1.0915	$(K, Na, Rb)(Li, Al, Fe)_3(Si, Al)_4O_{10}(F, OH)_2$	1.7287	$(Ag, Cu)_{16}(Sb, As)_2S_{11}$
1.0926	$NiMoO_4$	1.7321	$(Ag, Cu)_{16}As_2S_{11}$
1.0932	$AlCaMg_2(OH)_2(Al_{2.8}Si_{1.2})O_{10}$	1.7333	$(Ag, Cu)_{16}(Sb, As)_2(S, Se)_{11}$
1.0979	$Fe_3K(FeSi_3)O_{10}(OH)_2$	1.7340	$(Ag, Cu)_{16}(As, Sb)_2S_{11}$
1.0996	$KFe_3(FeSi_3)O_{10}(OH)_2$	1.7360	$CaK_3H(PO_4)_2$
1.0999	$(K_{0.95}Na_{0.05})(Mg_{2.80}Li_{0.20})(Si_{3.25}Al_{0.75})O_{10}F_2$	1.7396	$NaTiO_2$
1.0999	$K(MgLi)Si_4O_{10}F_2$	1.7460	$Li_2Si$
1.1001	$MnMoO_4$	1.8364	$(Fe, Mn)_2FP_4$
1.1024	$Fe_3KAlSi_3O_{10}(OH)_2$	1.8462	$(Mn, Fe, Mg, Ca)_2FP_4$
1.1031	$(Mg, Fe, Mn)_3K(OH, F)_2AlSi_3O_{10}$	1.8488	$K_{0.26}MoO_3$
1.1053	$(Al, Ca, Mg)_2(OH)(Si, Al)_2O_5$	1.9162	$Al_{13}Fe_4$
1.1080	$(Li, Fe, Al)_3K(F, OH)_2(Si, Al)_4O_{10}$	1.9203	$CrI_2$
1.1087	$KLi_2AlSi_4O_{10}(OH, F)_2$	1.9334	$Na_2Sb_4S_7$
1.1118	$Mg_3K(OH)_2AlSi_3O_{10}$	1.9372	$Al_{13}Ru_4$
1.1149	$Zn(N_2H_4)_2Cl_2$	1.9496	$CrBr_2$
1.1174	$[Mn(N_2H_4)_2]Cl_2$	1.9545	$NaNiO_2$
1.1181	$K(Mg, Fe)(Al, Fe)Si_4O_{10}(OH)_2$	1.9665	$Tl_2CO_3$
1.1188	$K_{1.30}Mg_{4.80}Li_{1.25}Si_{7.96}O_{20.03}F_{3.97}$	1.9976	$Sb_2O_3$
1.1206	$(K_{0.9}Mn_{0.1})Mg_3(Si_3Fe)O_{10}(OH)_2$	2.0303	$CuCl_2$
1.1224	$CaCuAlSi_2O_6(OH)_3$	2.0451	$CuMnO_2$
1.1240	$ALLi_2K(OH, F)_2AlSi_3O_{10}$	2.0524	$Al_2O_3$
1.1276	$KV_2AlSi_3O_{10}(OH)_2$	2.0636	$CuBr_2$
1.1308	$Fe_{17}Th_2$	2.1166	$Na_5Zr_2F_{13}$
1.1324	$(Na, K, Ba, Ca)(Ti, Mg, Fe, Nb)[(Si, Al)_2(O, OH)_7] \cdot H_2O$	2.1487	$K_{0.28}MoO_3$
1.1371	$Co_{17}Th_2$	2.1619	$Zn_5(OH)_6(O_3)_2$
1.1386	$(Fe, Mg)_2K(OH)_2(Al, Si)Si_3O_{10}$	2.1761	$Pb_2SO_4$
1.1742	$Cr_7Te_8$	2.1796	$Pb_2SO_4$
1.1927	$Cr_7Se_8$	2.2134	$BaTe(S_2O_3)_2 \cdot 2H_2O$
1.2031	$Ti_5Se_8$	2.3187	$Li_8Pb_3$
1.2094	$Na_2Co_5Mo_4Cl_4O_{16}$	2.3267	$ThTi_2O_6$
1.2126	$V_5Se_8$	2.3511	$UTi_2O_6$
1.2139	$Ni_4Pu$	2.3545	$NaMo_6O_{17}$
1.2153	$KMgCl(SO_4) \cdot 3H_2O$	2.3784	$Mg(UO_2)_2Si_2O_7 \cdot 6H_2O$
1.2211	$V_5S_8$	2.3942	$(Na, K)_5(Fe, Mn, Ca)_{16}(PO_4)_{12}(F, OH) \cdot H_2O$
1.2479	$CoCl_2 \cdot 6H_2O$	2.3961	$Ce_2Ti_2Si_2O_{11}$
1.2525	$K_2Mn(SO_4)_2 \cdot 4H_2O$	2.4094	$Mg(UO_2)_2(SiO_4)_2 \cdot 5H_2O$
1.3175	$Cu_2SO_4$	2.4235	$Ce_2Ti_2Si_2O_{11}$
1.3203	$Cu_2SO_4$	2.4774	$Pb(OH)Cl$
1.3394	$Sb_2SO_2$	2.5650	$Ti_3O_5$
1.3523	$Cu_2Na(OH)(SO_4)_2 \cdot H_2O$	2.7537	$Ge_2O_5$
1.3536	$Cu_2Na(OH)(SO_4)_2 \cdot H_2O$	2.7989	$(Ba, Sr, K)Na(Ti, Fe)TiSi_2(O, OH, F)_9$
1.3846	$MgCl_2 \cdot 6H_2O$	2.8981	$Ni_3Se_4$
1.3851	$MgBr_2 \cdot 6H_2O$	2.9976	$Bi_2Pd$
1.3927	$Ni(NH_3)_4(NCS)_2$	3.0434	$W_6P_2O_7$
1.3983	$CoO$	3.0577	$CoGe$
1.4142	$K_2TeCl_6$	3.2021	$Ag_{1-x}V_2O_5$
1.4275	$Al_4Be_5Fe_2$	3.2040	$AlNbO_4$
1.4277	$Ni(NH_3)_4(NO_2)_2$	3.2089	$Cr_2NiSe_4$
1.4847	$Cu(NH_3)_4(NO_2)_2$	3.2211	$Cr_2TiTe_4$
1.4988	$(Mg, Fe, Al)_{12}(OH)_{16}(Si, Al)_8O_{20}$	3.2222	$Ca_4(Fe, Mn, Mg)(Al, Fe)_5(OH)_3Si_6O_{23} \cdot 2H_2O$
1.5161	$(Mg, Fe, Al)_{12}(OH)_{16}(Si, Al)_8O_{20}$	3.2416	$V_{12}O_{26}$
1.5174	$(Mg, Fe, Al)_6(Si, Al)_4O_{10}(OH)_8$	3.2514	$Cr_3Se_4$
1.5206	$RbH_2P$	3.2569	$Cr_2NiS_4$
1.5214	$Al_2(PO_4)(OH)_3$	3.2573	$Cr_2NiS_4$
1.5410	$Li_4Ge_9O_{20}$	3.2796	$WV_2O_7$
1.5451	$(Al, Fe, Cr)Mg_5(OH)_8AlSi_3O_{10}$	3.2818	$(Al, Li)(OH)_2MnO_2$
1.5460	$Cs_2UO_2Cl_4$	3.2865	$Cr_3S_4$
1.5502	$NaCr_3O_8$	3.2882	$Cr_3S_4$
1.5543	$Al_2Mg_5Si_3O_{10}(OH)_8$	3.3241	$Al_{0.32}V_2O_5$
1.5558	$(NH_4)_2SbCl_5$	3.3255	$TiCr_2S_4$
1.5647	$KH_2P$	3.3272	$FeHo_4S_7$
1.5677	$KCr_3O_8$	3.3300	$FeY_4S_7$
1.5685	$TlCr_3O_8$	3.3300	$CrDy_4Se_7$
1.5716	$(NH_4)_2S_2O_3$	3.3306	$MnYb_4S_7$

C2/m C<sub>2h</sub><sup>3</sup> No. 12 (continued)

## Inorganic (continued)

3.3331	MnDy <sub>4</sub> S <sub>7</sub>	3.7512	Ba(NCS) <sub>2</sub> •2H <sub>2</sub> O
3.3336	FeEr <sub>4</sub> S <sub>7</sub>	3.7772	Al <sub>13</sub> Ge <sub>4</sub>
3.3340	MnY <sub>4</sub> S <sub>7</sub>	3.9023	Sm <sub>2</sub> Ge <sub>3</sub>
3.3340	MnTm <sub>4</sub> S <sub>7</sub>	3.9332	Cf <sub>2</sub> Ge <sub>3</sub>
3.3350	FeDy <sub>4</sub> Se <sub>7</sub>	3.9526	TaTe <sub>2</sub>
3.3354	V <sub>3</sub> Te <sub>4</sub>	3.9662	NbTe <sub>2</sub>
3.3355	FeYb <sub>4</sub> S <sub>7</sub>	3.9816	Na <sub>2</sub> Ti <sub>6</sub> Ge <sub>13</sub>
3.3366	FeTm <sub>4</sub> S <sub>7</sub>	4.0230	Ge <sub>2</sub> Ge <sub>3</sub>
3.3378	MnHo <sub>4</sub> S <sub>7</sub>	4.0546	AgBi <sub>3</sub> S <sub>5</sub>
3.3378	MnEr <sub>4</sub> S <sub>7</sub>	4.0578	Al <sub>4</sub> Li <sub>9</sub>
3.3392	MnDy <sub>4</sub> Se <sub>7</sub>	4.0702	H <sub>6</sub> V <sub>4</sub> Ge <sub>10</sub>
3.3415	CoV <sub>2</sub> S <sub>4</sub>	4.0791	K <sub>2</sub> Ti <sub>6</sub> Ge <sub>13</sub>
3.3429	Nb <sub>2</sub> Ge <sub>5</sub>	4.1053	K <sub>2</sub> Ti <sub>6</sub> Ge <sub>13</sub>
3.3530	Dy <sub>5</sub> S <sub>7</sub>	4.1113	AsGe
3.3533	Ho <sub>5</sub> S <sub>7</sub>	4.1944	Li <sub>0.30</sub> V <sub>2</sub> Ge <sub>5</sub>
3.3566	Er <sub>5</sub> S <sub>7</sub>	4.2494	K <sub>0.33</sub> V <sub>2</sub> Ge <sub>5</sub>
3.3573	Y <sub>5</sub> S <sub>7</sub>	4.2494	N <sub>0.33</sub> V <sub>2</sub> Ge <sub>5</sub>
3.3576	Tm <sub>5</sub> S <sub>7</sub>	4.2982	BaTi <sub>2</sub> Ge <sub>5</sub>
3.3605	NiV <sub>2</sub> Se <sub>4</sub>	4.3463	Nb <sub>7</sub> P <sub>4</sub>
3.3626	Co(NH <sub>3</sub> ) <sub>5</sub> N <sub>6</sub> Br <sub>2</sub> •2H <sub>2</sub> O	4.3563	AsSi
3.3689	NiV <sub>2</sub> S <sub>4</sub>	4.4828	Sb <sub>8</sub> Ge <sub>10</sub> (OH) <sub>2</sub> Cl <sub>2</sub>
3.3823	NiV <sub>2</sub> S <sub>4</sub>	4.4911	BiCu <sub>2</sub> S <sub>2</sub>
3.3982	As <sub>3</sub> W <sub>2</sub>	4.5098	Sb <sub>8</sub> Ge <sub>10</sub> (OH) <sub>2</sub> Br <sub>2</sub>
3.4333	FeV <sub>2</sub> S <sub>4</sub>	4.5242	Sb <sub>8</sub> Ge <sub>10</sub> (OH) <sub>2</sub> I <sub>2</sub>
3.4506	(Ba, Pb, K, Na) <sub>1.02</sub> (Mn, Mn, Fe, Al, Si) <sub>7.86</sub> (OH) <sub>1.6</sub>	4.6588	TiNb <sub>2</sub> Ge <sub>7</sub>
3.4568	NaOH•4H <sub>2</sub> O	4.8090	(Ba, H <sub>2</sub> O) <sub>2</sub> Mn <sub>5</sub> Ge <sub>10</sub>
3.4612	As <sub>3</sub> Mo <sub>2</sub>	5.8425	NaNb <sub>13</sub> Ge <sub>33</sub>
3.4665	V <sub>3</sub> S <sub>4</sub>	6.3746	V <sub>3</sub> Ge <sub>4</sub> (OH) <sub>4</sub>
3.6750	Bi <sub>5</sub> Cu <sub>3</sub> S <sub>9</sub>	7.4175	Bi <sub>24</sub> Ge <sub>31</sub> Cl <sub>10</sub>
3.7091	P <sub>4</sub> Re <sub>3</sub>	7.4775	Bi <sub>24</sub> Ge <sub>31</sub> Br <sub>10</sub>

## Organic

0.5180	C <sub>37</sub> H <sub>43</sub> FeN <sub>4</sub> O <sub>5</sub>	1.2237	Cu(NH <sub>3</sub> ) <sub>4</sub> (SCN) <sub>2</sub>
0.5673	C <sub>4</sub> H <sub>16</sub> B <sub>2</sub> N <sub>2</sub>	1.3067	(CH <sub>3</sub> PS <sub>2</sub> ) <sub>2</sub>
0.6041	Co(NCS) <sub>2</sub> •2C <sub>5</sub> NH <sub>5</sub>	1.3454	C <sub>7</sub> H <sub>7</sub> S <sub>2</sub> SK•H <sub>2</sub> O
0.6384	[(CH <sub>3</sub> ) <sub>2</sub> C:C:Ge] <sub>2</sub>	1.3706	C <sub>6</sub> H <sub>4</sub> (NC) <sub>2</sub>
0.6401	Cu(NCS) <sub>2</sub> •2C <sub>5</sub> NH <sub>5</sub>	1.3927	Ni(NH <sub>3</sub> ) <sub>4</sub> (NCS) <sub>2</sub>
0.6466	Fe(C <sub>5</sub> H <sub>4</sub> OCOC <sub>6</sub> H <sub>4</sub> F) <sub>2</sub>	1.4868	C <sub>3</sub> H <sub>7</sub> C <sub>6</sub> OH
0.6636	Ca <sub>7</sub> (Si <sub>3</sub> ) <sub>6</sub> (C <sub>6</sub> ) <sub>3</sub> •2H <sub>2</sub> O	1.5090	Rb <sub>2</sub> C <sub>6</sub> Ge <sub>6</sub>
0.6805	SrNi(CN) <sub>4</sub> •5H <sub>2</sub> O	1.6033	C <sub>12</sub> H <sub>24</sub>
0.6845	SrPt(CN) <sub>4</sub> •5H <sub>2</sub> O	1.6074	H <sub>6</sub> CH <sub>2</sub> •C <sub>6</sub> GeLi•H <sub>2</sub> O
0.6860	SrPd(CN) <sub>4</sub> •5H <sub>2</sub> O	1.6833	Na <sub>2</sub> Ni(CN) <sub>4</sub> •3H <sub>2</sub> O
0.6991	(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> Ni(AgBr <sub>2</sub> ) <sub>2</sub>	1.7664	Ni(C <sub>6</sub> H <sub>4</sub> CCH <sub>3</sub> ) <sub>2</sub> •2H <sub>2</sub> O
0.7773	(NC) <sub>2</sub> C=C <sub>6</sub> H <sub>4</sub> =C(CN) <sub>2</sub> •(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	1.8273	GeCl <sub>4</sub> (N:CHCH:CH:CH:CH) <sub>2</sub>
0.7809	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> Ge <sub>3</sub> H <sub>2</sub> O	1.8275	2(ICl) <sub>2</sub> •C <sub>4</sub> H <sub>8</sub> Ge <sub>2</sub>
0.7863	C <sub>14</sub> H <sub>8</sub> Cl <sub>4</sub>	1.8538	(CH <sub>3</sub> •C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> CrI
0.8597	KNaPt(CN) <sub>4</sub> •3H <sub>2</sub> O	1.8922	C <sub>16</sub> H <sub>10</sub> N <sub>2</sub> Ge <sub>2</sub>
0.8606	C <sub>6</sub> H <sub>6</sub> •Cl <sub>2</sub>	1.9665	Tl <sub>2</sub> C <sub>6</sub> Ge <sub>3</sub>
0.8777	C <sub>6</sub> H <sub>6</sub> Br <sub>2</sub>	2.0992	BaSe(S <sub>2</sub> Ge <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> O•0.5C <sub>4</sub> H <sub>8</sub> Ge <sub>2</sub>
1.0559	C <sub>3</sub> H <sub>7</sub> NH <sub>3</sub> Cl	2.1619	Zn <sub>5</sub> (OH) <sub>6</sub> (C <sub>6</sub> ) <sub>2</sub>
1.0600	C <sub>4</sub> H <sub>8</sub> Ge <sub>2</sub> •Cl <sub>2</sub>	3.3172	C <sub>6</sub> H <sub>5</sub> Cl <sub>2</sub> Tl
1.0663	(C <sub>4</sub> H <sub>8</sub> Ge <sub>2</sub> )Br <sub>2</sub>	3.4905	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> Ge <sub>2</sub> Ni
1.1085	NiBr <sub>2</sub> ([CH <sub>3</sub> ] <sub>2</sub> C <sub>4</sub> H <sub>2</sub> N <sub>2</sub> )	3.6588	(C <sub>6</sub> H <sub>2</sub> )Cl(N <sub>6</sub> ) <sub>3</sub>
1.1232	[(CH <sub>3</sub> ) <sub>2</sub> NBF <sub>2</sub> ] <sub>2</sub>	3.7512	Ba(NCS) <sub>2</sub> •2H <sub>2</sub> O
1.1484	[HCl <sub>2</sub> •N(CH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub>	8.6510	C <sub>17</sub> H <sub>35</sub> C <sub>6</sub> GeNa•0.125H <sub>2</sub> O
1.1548	(CH <sub>3</sub> ) <sub>3</sub> N <sub>6</sub>		

2  
mP2/c C<sub>2h</sub><sup>4</sup> No. 13Inorganic - 56  
Organic - 42

## Inorganic

0.6529	S	0.8662	MgW <sub>6</sub>
0.7060	[(Mg, Al) <sub>5</sub> (Si, Al) <sub>8</sub> Ge <sub>20</sub> (OH) <sub>2</sub> •8H <sub>2</sub> O]	0.8671	FeW <sub>6</sub>
0.8537	ZnMo <sub>6</sub>	0.8675	NiW <sub>6</sub>
0.8589	NiMo <sub>6</sub>	0.8680	CoW <sub>6</sub>
0.8589	CoMo <sub>6</sub>	0.8688	FeMo <sub>6</sub>
0.8617	MgMo <sub>6</sub>	0.8691	(Fe, Mn)W <sub>6</sub>
0.8626	MnMo <sub>6</sub>	0.8693	MgW <sub>6</sub>
0.8628	MnW <sub>6</sub>	0.8693	NiW <sub>6</sub>
0.8639	ZnW <sub>6</sub>	0.8699	FeW <sub>6</sub>
0.8660	CdW <sub>6</sub>	0.8896	FeNb <sub>6</sub>

P2/c  $C_{2h}^4$  No. 13 (continued)

## Inorganic (continued)

0.8912	InNb $\sigma_4$	1.6052	Na <sub>2</sub> B <sub>4</sub> $\sigma_7 \cdot 4H_2\sigma$
0.8930	InTa $\sigma_4$	1.6204	Na <sub>2</sub> B <sub>4</sub> $\sigma_7 \cdot 4H_2\sigma$
0.9004	ScNb $\sigma_4$	1.9082	InF <sub>3</sub> $\sigma_3H_2\sigma$
0.9026	ScTa $\sigma_4$	1.9101	(Fe, Mn) <sub>5</sub> H <sub>2</sub> (P $\sigma_4$ ) <sub>4</sub> $\cdot 4H_2\sigma$
0.9978	Na <sub>2</sub> S <sub>2</sub> $\sigma_4$	1.9205	Mn <sub>5</sub> H <sub>2</sub> (P $\sigma_4$ ) <sub>4</sub> $\cdot 4H_2\sigma$
1.0712	BaK <sub>2</sub> (S <sub>6</sub> $\sigma_6$ ) <sub>2</sub>	1.9955	AgAuTe <sub>4</sub>
1.1227	Ca[B( $\sigma H$ ) <sub>4</sub> ] <sub>2</sub>	2.1201	Zn <sub>4</sub> ( $\sigma H$ ) <sub>2</sub> (P $\sigma_4$ ) <sub>2</sub> $\cdot 3H_2\sigma$
1.1894	Ca[B( $\sigma H$ ) <sub>4</sub> ] <sub>2</sub> $\cdot 2H_2\sigma$	2.2023	LiAlSi <sub>4</sub> $\sigma_{10}$
1.4763	GdCl <sub>3</sub> $\cdot 6H_2\sigma$	2.2359	B <sub>10</sub> H <sub>14</sub>
1.4763	SmCl <sub>3</sub> $\cdot 6H_2\sigma$	2.3124	Ca <sub>6</sub> ( $\sigma H$ ) <sub>2</sub> (Si <sub>6</sub> $\sigma_{17}$ )
1.4791	ErCl <sub>3</sub> $\cdot 6H_2\sigma$	2.3545	P
1.4791	GdCl <sub>3</sub> $\cdot 6H_2\sigma$	2.5225	Na <sub>4</sub> MnTi(Zr <sub>1.5</sub> Ti <sub>0.5</sub> ) $\sigma_2$ (F, $\sigma H$ ) <sub>2</sub> (Si <sub>2</sub> $\sigma_7$ ) <sub>2</sub>
1.4793	TbCl <sub>3</sub> $\cdot 6H_2\sigma$	3.7262	Na <sub>4</sub> Ge <sub>5</sub> Sn <sub>2</sub> $\sigma_{15}$ ( $\sigma H$ ) <sub>2</sub>
1.4806	TmCl <sub>3</sub> $\cdot 6H_2\sigma$	4.1563	Mo $\sigma_{26}$
1.4807	HoCl <sub>3</sub> $\cdot 6H_2\sigma$	4.1584	Mo $\sigma_{23}$
1.4807	DyCl <sub>3</sub> $\cdot 6H_2\sigma$	4.3750	(Mo, W) <sub>10</sub> $\sigma_{29}$
1.4824	EuCl <sub>3</sub> $\cdot 6H_2\sigma$	4.6750	(Mo, W) <sub>11</sub> $\sigma_{32}$
1.5624	(NH <sub>4</sub> ) <sub>2</sub> Se(S $\sigma_3$ ) <sub>2</sub>	15.4433	W $\sigma_{2.96}$

## Organic

0.3129	CH <sub>3</sub> C $\sigma\sigma$ $\cdot\sigma Bi$	3.5214	C <sub>30</sub> H <sub>14</sub>
0.3441	C <sub>2</sub> H <sub>2</sub> I <sub>2</sub>	3.5333	C <sub>6</sub> H <sub>5</sub> $\sigma$ C <sub>4</sub> H <sub>5</sub> $\sigma$
0.9686	Pd(C <sub>12</sub> H <sub>10</sub> N <sub>3</sub> $\sigma$ ) <sub>2</sub>	3.5597	[(CH <sub>3</sub> ) <sub>2</sub> SiNH] <sub>4</sub>
1.2875	Cu[ $\sigma$ C <sub>6</sub> H <sub>4</sub> $\cdot\sigma CH:N\sigma C_6H_4$ ] <sub>2</sub> $\cdot 0.25(CHCl_3)$	3.6740	C <sub>5</sub> N <sub>4</sub> H <sub>3</sub> NH <sub>2</sub> $\cdot\sigma HCl$ $\cdot 0.5H_2\sigma$
1.7641	Si <sub>4</sub> C <sub>11</sub> H <sub>28</sub>	3.7146	C <sub>3</sub> $\sigma_2S_3$
1.7715	CCl <sub>3</sub> CH( $\sigma H$ ) <sub>2</sub>	3.9550	Cu(C <sub>9</sub> H <sub>6</sub> N $\sigma$ ) <sub>2</sub>
1.7937	C <sub>8</sub> H <sub>12</sub> $\cdot 2Ni\sigma$ (CH <sub>3</sub> ) <sub>4</sub> C <sub>6</sub> $\sigma_2$	3.9867	C <sub>6</sub> H <sub>6</sub> $\sigma_5$
1.8926	Rb[Fe(H $\sigma_2$ )( $\sigma\sigma C\sigma CH_2$ ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(CH <sub>2</sub> C $\sigma\sigma$ ) <sub>2</sub> ] $\cdot H_2\sigma$	4.0923	H $\sigma C_6H_4\sigma$ CH(C <sub>2</sub> H <sub>5</sub> ) $\cdot$ CH(C <sub>2</sub> H <sub>5</sub> ) $\cdot$ C <sub>6</sub> H <sub>4</sub> $\sigma H$
2.0105	(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> AsI <sub>3</sub>	4.2123	C <sub>14</sub> H <sub>11</sub> $\sigma_6$ Rb $\cdot H_2\sigma$
2.1117	C <sub>5</sub> H <sub>5</sub> FeC <sub>5</sub> H <sub>4</sub> $\cdot\sigma C\sigma$ C <sub>5</sub> H <sub>4</sub> FeC <sub>5</sub> H <sub>5</sub>	4.2932	C <sub>14</sub> H <sub>11</sub> K $\sigma_6$ H <sub>2</sub> $\sigma$
2.1167	[(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> P] <sub>2</sub> NiCl <sub>2</sub>	4.5828	(ClC <sub>6</sub> H <sub>4</sub> C $\sigma$ ) <sub>2</sub> $\sigma$
2.1716	C <sub>5</sub> H <sub>5</sub> FeC <sub>5</sub> H <sub>4</sub> $\cdot\sigma C\sigma$ C <sub>5</sub> H <sub>4</sub> RuC <sub>5</sub> H <sub>5</sub>	4.9173	C <sub>19</sub> H <sub>13</sub> BrN <sub>2</sub>
2.1883	[Cu(NC-CH <sub>2</sub> CH <sub>2</sub> -CN) <sub>2</sub> ] $\cdot N\sigma_3$	5.2265	C <sub>6</sub> H <sub>7</sub> BrS <sub>2</sub> $\cdot 0.5H_2\sigma$
2.1963	AgN $\sigma_3$ C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	5.2678	CoCl <sub>2</sub> (C <sub>5</sub> H <sub>5</sub> N) <sub>2</sub>
2.2792	C <sub>6</sub> H <sub>10</sub> $\sigma_4$	5.6406	HgCl <sub>2</sub> $\cdot$ C <sub>14</sub> H <sub>14</sub> N <sub>2</sub> $\sigma_3 \cdot 0.5C_3H_6\sigma$
2.3549	K[Cr(C <sub>2</sub> $\sigma_4$ ) <sub>2</sub> (H <sub>2</sub> $\sigma$ ) <sub>2</sub> ] $\cdot 3H_2\sigma$	7.4674	CB <sub>3</sub> (CH <sub>2</sub> ) <sub>15</sub> CHBrC $\sigma\sigma H$
2.4219	[(H <sub>2</sub> N) <sub>2</sub> CS] <sub>2</sub> Br <sub>2</sub> $\cdot H_2\sigma$	7.4732	C <sub>19</sub> H <sub>14</sub>
2.5371	C <sub>14</sub> H <sub>14</sub> $\sigma_3$ N <sub>2</sub>	7.5490	C <sub>16</sub> H <sub>33</sub> $\sigma H$
2.8617	CH <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	8.3860	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>7</sub> C $\sigma$ C(CH <sub>2</sub> ) <sub>7</sub> C $\sigma\sigma H$
3.1913	C <sub>26</sub> H <sub>32</sub> $\sigma_{14}Cl_2$	8.8294	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>16</sub> C $\sigma\sigma H$
3.4622	C <sub>7</sub> H <sub>5</sub> $\sigma_6$ N <sub>3</sub>	10.1592	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>7</sub> C $\sigma$ C(CH <sub>2</sub> ) <sub>11</sub> C $\sigma\sigma H$

 $\frac{2}{m}$ P2<sub>1</sub>/c  $C_{2h}^5$  No. 14Inorganic - 588  
Organic - 1783

## Inorganic

0.2094	Ni(N $\sigma_3$ ) <sub>2</sub> $\cdot 4H_2\sigma$	0.4696	SeS <sub>2</sub> N <sub>2</sub> Cl <sub>5</sub>
0.2552	Ag <sub>5</sub> Ba <sub>2</sub> (N $\sigma_2$ ) <sub>9</sub> $\cdot 0.5H_2\sigma$	0.4759	NH <sub>4</sub> Nd(S $\sigma_4$ ) <sub>2</sub> $\cdot 4H_2\sigma$
0.2626	Na <sub>3</sub> HP <sub>2</sub> $\sigma_7 \cdot 9H_2\sigma$	0.4839	(N <sub>2</sub> H $\sigma$ ) <sub>3</sub> CdCl <sub>5</sub>
0.2807	(NH <sub>4</sub> ) <sub>6</sub> Mo $\sigma_7 \sigma_{24} \cdot 4H_2\sigma$	0.4862	Bi $\sigma H$ Se $\sigma_4 \cdot H_2\sigma$
0.2877	H <sub>5</sub> I $\sigma_6$	0.4882	Bi $\sigma H$ Se $\sigma_4 \cdot 0.5H_2\sigma$
0.3030	NH <sub>4</sub> Ag(SCN) <sub>2</sub>	0.4945	AuCl $\cdot$ PCL <sub>3</sub>
0.3333	AlBe( $\sigma H$ )Si $\sigma_4$	0.4948	Bi $\sigma H$ S $\sigma_4 \cdot H_2\sigma$
0.3483	Mg <sub>2</sub> Al <sub>4</sub> $\sigma_6$ (Si $\sigma_4$ )	0.5100	P <sub>4</sub> S <sub>7</sub>
0.3489	Na <sub>2</sub> S <sub>2</sub> $\sigma_3 \cdot 5H_2\sigma$	0.5117	KF $\cdot 4H_2\sigma$
0.3582	Mg <sub>3</sub> (P $\sigma_4$ ) <sub>2</sub> $\cdot 8H_2\sigma$	0.5194	Mg(N $\sigma_3$ ) <sub>2</sub> $\cdot 6H_2\sigma$
0.3627	(Mn, Mg) <sub>3</sub> (As $\sigma_4$ ) <sub>2</sub> $\cdot 8H_2\sigma$	0.5217	Mg(N $\sigma_3$ ) <sub>2</sub> $\cdot 6H_2\sigma$
0.3652	(Mg, Fe)(Ce, La, Nd, Pr) <sub>2</sub> (C $\sigma_3$ ) <sub>4</sub>	0.5468	AgCN $\cdot 2AgN\sigma_3$
0.3734	Be(Mn, Fe)( $\sigma H$ )P $\sigma_4$	0.5514	Bi $\sigma_2 \sigma_2$ S $\sigma_4 \cdot H_2\sigma$
0.3782	PbN <sub>2</sub> S <sub>2</sub> $\cdot NH_3$	0.5554	Bi $\sigma_2 \sigma_2$ Se $\sigma_4 \cdot H_2\sigma$
0.4001	Cu <sub>3</sub> ( $\sigma H$ ) <sub>2</sub> (Mo $\sigma_4$ ) <sub>2</sub>	0.5556	HCl $\cdot 2H_2\sigma$
0.4070	As $\sigma_2 \sigma_3$	0.5580	Pb <sub>4</sub> ( $\sigma H$ ) <sub>2</sub> (C $\sigma_3$ ) <sub>2</sub> S $\sigma_4$
0.4079	As $\sigma_2 \sigma_3$	0.5700	(Fe, Mn, Mg) <sub>13</sub> (Fe, Al) <sub>7</sub> Si <sub>13</sub> $\sigma_{44}$ ( $\sigma H$ ) <sub>11</sub>
0.4112	As $\sigma_2 \sigma_3$	0.5748	PhAgAsS <sub>3</sub>
0.4320	As $\sigma_3$ SbS <sub>3</sub>	0.5811	MgS $\sigma_4 \cdot 4H_2\sigma$
0.4375	Ca <sub>2</sub> (Co, Mg)(As $\sigma_4$ ) <sub>2</sub> $\cdot 2H_2\sigma$	0.5821	MnS $\sigma_4 \cdot 4H_2\sigma$
0.4414	Ca <sub>2</sub> Mn(As $\sigma_4$ ) <sub>2</sub> $\cdot 2H_2\sigma$	0.5826	CoS $\sigma_4 \cdot 4H_2\sigma$
0.4469	Na $\sigma H$ $\cdot 7H_2\sigma$	0.5843	FeS $\sigma_4 \cdot 4H_2\sigma$
0.4501	AsFeS	0.5853	ZnS $\sigma_4 \cdot 4H_2\sigma$
0.4580	CuNa <sub>2</sub> (S $\sigma_4$ ) <sub>2</sub> $\cdot 2H_2\sigma$	0.5853	Al( $\sigma H$ ) <sub>3</sub>
0.4640	(NH <sub>4</sub> ) <sub>2</sub> Ce(S $\sigma_4$ ) <sub>2</sub> $\cdot 4H_2\sigma$	0.5864	NiS $\sigma_4 \cdot 4H_2\sigma$

P2<sub>1</sub>/c C<sub>2h</sub><sup>5</sup> No. 14 (continued)

## Inorganic (continued)

0.5872	FeMg(OH)(SO <sub>4</sub> ) <sub>2</sub> •7H <sub>2</sub> O	0.7676	CuSnF <sub>6</sub> •4H <sub>2</sub> O
0.5886	FeZn(OH)(SO <sub>4</sub> ) <sub>2</sub> •7H <sub>2</sub> O	0.7714	NaHCO <sub>3</sub>
0.5887	PbAgSbS <sub>3</sub>	0.7742	NaHCO <sub>3</sub>
0.5888	(Zn, Mn, Mg, Fe)Fe(SO <sub>4</sub> ) <sub>2</sub> (OH)•7H <sub>2</sub> O	0.7762	CaB <sub>3</sub> O <sub>4</sub> (OH) <sub>3</sub> •H <sub>2</sub> O
0.5894	KNa <sub>3</sub> H <sub>3</sub> [Cu(IO <sub>6</sub> ) <sub>2</sub> ]•14H <sub>2</sub> O	0.7769	(UO <sub>2</sub> ) <sub>2</sub> H <sub>11</sub> (PO <sub>4</sub> ) <sub>5</sub>
0.5951	AuCl <sub>3</sub>	0.7780	UO <sub>2</sub> (H <sub>2</sub> PO <sub>4</sub> ) <sub>2</sub> •3H <sub>2</sub> O
0.5965	MgCl <sub>2</sub> •12H <sub>2</sub> O	0.7793	B <sub>10</sub> H <sub>16</sub>
0.5980	K <sub>2</sub> LiF <sub>3</sub> •9H <sub>2</sub> O	0.7794	BiOHCrO <sub>4</sub>
0.5988	Na <sub>2</sub> CuF <sub>4</sub>	0.7822	Na <sub>4</sub> P <sub>4</sub> O <sub>12</sub> •4H <sub>2</sub> O
0.6072	Ba(BO <sub>2</sub> ) <sub>2</sub> •4H <sub>2</sub> O	0.7880	Cu <sub>2</sub> (OH) <sub>2</sub> CO <sub>3</sub>
0.6105	Cu(ClO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.7965	BaSi <sub>2</sub> O <sub>5</sub> •3H <sub>2</sub> O
0.6120	H <sub>4</sub> Fe(CN) <sub>6</sub>	0.7972	KAuBr <sub>4</sub> •2H <sub>2</sub> O
0.6135	NaCN•2H <sub>2</sub> O	0.7973	Na <sub>2</sub> BiI <sub>5</sub> •4H <sub>2</sub> O
0.6136	2H <sub>3</sub> PO <sub>4</sub> •H <sub>2</sub> O	0.8045	H <sub>3</sub> GeClO <sub>4</sub>
0.6143	(NH <sub>4</sub> ) <sub>2</sub> Te(S <sub>2</sub> O <sub>3</sub> ) <sub>2</sub>	0.8055	HB <sub>2</sub>
0.6176	Na <sub>2</sub> Mn <sub>2</sub> Si <sub>2</sub> O <sub>7</sub>	0.8077	K <sub>3</sub> Fe(CN) <sub>6</sub>
0.6187	SrB <sub>2</sub> O <sub>4</sub> •4H <sub>2</sub> O	0.8077	K <sub>3</sub> Co(CN) <sub>6</sub>
0.6248	Sr[B(OH) <sub>4</sub> ] <sub>2</sub>	0.8099	Rh <sub>3</sub> Fe(CN) <sub>6</sub>
0.6257	NaOH•5H <sub>2</sub> O	0.8116	KZnBr <sub>3</sub> •2H <sub>2</sub> O
0.6337	KCuCl <sub>3</sub>	0.8125	HB <sub>2</sub>
0.6345	NH <sub>4</sub> CuCl <sub>3</sub>	0.8201	Na <sub>4</sub> UO <sub>2</sub> (O <sub>2</sub> ) <sub>3</sub> •9H <sub>2</sub> O
0.6353	Np <sub>2</sub> O <sub>5</sub>	0.8203	FePb <sub>4</sub> Sb <sub>6</sub> S <sub>14</sub>
0.6389	Ti(NO <sub>3</sub> ) <sub>4</sub>	0.8205	LiCuCl <sub>3</sub> •2H <sub>2</sub> O
0.6395	KCuCl <sub>3</sub>	0.8248	FePb <sub>4</sub> Sb <sub>6</sub> S <sub>14</sub>
0.6404	CaC <sub>2</sub> O <sub>4</sub> •H <sub>2</sub> O	0.8253	CaK <sub>4</sub> (Mo <sub>7</sub> O <sub>24</sub> )•7H <sub>2</sub> O
0.6414	Ce(IO <sub>3</sub> ) <sub>4</sub> •H <sub>2</sub> O	0.8264	CuHgO(NO <sub>3</sub> ) <sub>2</sub> •3H <sub>2</sub> O
0.6432	Ca(IO <sub>3</sub> ) <sub>2</sub>	0.8280	Cs <sub>2</sub> Ge <sub>5</sub> O <sub>11</sub>
0.6461	NaBr•2H <sub>2</sub> O	0.8351	Mn <sub>7</sub> (OH) <sub>8</sub> (AsO <sub>4</sub> ) <sub>2</sub>
0.6480	NaBr•2H <sub>2</sub> O	0.8407	B <sub>2</sub> F <sub>4</sub>
0.6532	NaBr•2H <sub>2</sub> O	0.8428	CuCN•NH <sub>3</sub>
0.6571	BaCl <sub>2</sub> •2H <sub>2</sub> O	0.8560	B <sub>4</sub> H <sub>10</sub>
0.6584	BaCl <sub>2</sub> •2H <sub>2</sub> O	0.8615	HgCrO <sub>4</sub>
0.6592	Rb <sub>2</sub> PuF <sub>7</sub>	0.8618	AgMnO <sub>4</sub>
0.6646	Al <sub>2</sub> (OH) <sub>2</sub> (H <sub>2</sub> O) <sub>8</sub> (SeO <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> O	0.8683	CoSeO <sub>3</sub> •2H <sub>2</sub> O
0.6676	K <sub>4</sub> (HSiO <sub>3</sub> ) <sub>4</sub>	0.8693	ZnSeO <sub>3</sub> •2H <sub>2</sub> O
0.6708	K <sub>2</sub> NbF <sub>7</sub>	0.8731	CaB <sub>3</sub> O <sub>3</sub> (OH) <sub>5</sub> •4H <sub>2</sub> O
0.6726	CaB <sub>6</sub> O <sub>10</sub> •5H <sub>2</sub> O	0.8733	RuNO(OH)(NO <sub>2</sub> ) <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub>
0.6732	Al <sub>2</sub> (OH) <sub>2</sub> (H <sub>2</sub> O) <sub>8</sub> (SO <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> O	0.8779	BaO <sub>2</sub> •H <sub>2</sub> O <sub>2</sub>
0.6783	CaC <sub>2</sub> O <sub>4</sub> •H <sub>2</sub> O	0.8800	B <sub>2</sub> H <sub>6</sub>
0.6867	AsS	0.8825	CoNb <sub>2</sub> O <sub>6</sub>
0.6886	Mg <sub>7</sub> Al <sub>18</sub> Si <sub>3</sub> O <sub>40</sub>	0.8829	FePO <sub>4</sub> •2H <sub>2</sub> O
0.7068	Na <sub>2</sub> Si <sub>3</sub> O <sub>8</sub> •8H <sub>2</sub> O	0.8846	NiNb <sub>2</sub> O <sub>6</sub>
0.7109	Fe <sub>4</sub> (SO <sub>4</sub> ) <sub>6</sub> •15H <sub>2</sub> O	0.8858	SbOCl
0.7308	HfF <sub>4</sub> •3H <sub>2</sub> O	0.8874	(Sr, Ca) <sub>2</sub> B <sub>14</sub> O <sub>23</sub> •8H <sub>2</sub> O
0.7344	(NH <sub>4</sub> ) <sub>2</sub> Ni(BeF <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.8875	FePO <sub>4</sub> •2H <sub>2</sub> O
0.7349	Ni(NH <sub>4</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.8913	Zn <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>
0.7356	Cd(NH <sub>4</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.8942	AlPO <sub>4</sub> •2H <sub>2</sub> O
0.7363	K <sub>2</sub> Pd(NO <sub>2</sub> ) <sub>4</sub>	0.8953	Mg(B <sub>4</sub> O <sub>7</sub> (OH) <sub>6</sub> )•6H <sub>2</sub> O
0.7367	(NH <sub>4</sub> ) <sub>2</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9010	Ca(UO <sub>2</sub> Si <sub>3</sub> O <sub>8</sub> (OH)) <sub>2</sub> •5H <sub>2</sub> O
0.7367	Ni(NH <sub>4</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9015	FeOHCl
0.7376	Mn(NH <sub>4</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9030	LiNH <sub>4</sub> SiF <sub>6</sub>
0.7379	Zn(NH <sub>4</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9059	XeF <sub>2</sub> •XeF <sub>4</sub>
0.7379	K <sub>2</sub> Ni(SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9140	ZnOHCl
0.7383	Fe(NH <sub>4</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9160	Cu(OH)Cl
0.7383	Zn(NH <sub>4</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9169	Mn <sub>3</sub> /2Fe <sub>1</sub> /2(OH)PO <sub>4</sub>
0.7386	K <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9173	Pb <sub>5</sub> Sb <sub>4</sub> S <sub>11</sub>
0.7386	Co(NH <sub>4</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9189	Bi <sub>2</sub> O <sub>3</sub>
0.7402	Mg(NH <sub>4</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9191	NH <sub>4</sub> OH
0.7406	Mg(NH <sub>4</sub> ) <sub>2</sub> (SeO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9196	Mg <sub>2</sub> B <sub>2</sub> O <sub>11</sub> •15H <sub>2</sub> O
0.7416	Cu(NH <sub>4</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9216	(Mn, Fe) <sub>2</sub> (OH)(PO <sub>4</sub> )
0.7424	MgTi <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9231	KICl <sub>4</sub>
0.7429	K <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9241	K <sub>2</sub> [Pt(NO <sub>2</sub> ) <sub>4</sub> Cl <sub>2</sub> ]
0.7446	Cu(NH <sub>4</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9255	KICl <sub>4</sub> •H <sub>2</sub> O
0.7452	CuSiF <sub>6</sub> •4H <sub>2</sub> O	0.9263	(Fe, Mn) <sub>2</sub> (OH)PO <sub>4</sub>
0.7456	Cu(NH <sub>4</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> O	0.9270	Pb <sub>5</sub> Sb <sub>4</sub> S <sub>11</sub>
0.7507	CuHfF <sub>6</sub> •4H <sub>2</sub> O	0.9328	Cl <sub>6</sub> Si <sub>2</sub> O
0.7507	CuZrF <sub>6</sub> •4H <sub>2</sub> O	0.9363	Mn <sub>2</sub> (OH)(AsO <sub>4</sub> )
0.7553	CuTiF <sub>6</sub> •4H <sub>2</sub> O	0.9420	CaBe <sub>2</sub> P <sub>2</sub> O <sub>8</sub>
0.7558	(Fe, Mn, Ca) <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>	0.9435	Ca[Al <sub>2</sub> Si <sub>2</sub> O <sub>8</sub> ] <sub>2</sub> •4H <sub>2</sub> O
0.7567	CuNbOF <sub>5</sub> •4H <sub>2</sub> O	0.9471	Ba(AlSiO <sub>4</sub> ) <sub>2</sub>
0.7583	CuWO <sub>2</sub> F <sub>4</sub> •4H <sub>2</sub> O	0.9495	B <sub>18</sub> H <sub>22</sub>
0.7587	Ca(CH <sub>3</sub> COO)Cl•5H <sub>2</sub> O	0.9512	Mg <sub>2</sub> FP <sub>4</sub>
0.7666	(Fe, Mn, Ca) <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>	0.9557	(NH <sub>4</sub> ) <sub>2</sub> Ca <sub>3</sub> (P <sub>2</sub> O <sub>7</sub> ) <sub>2</sub> •6H <sub>2</sub> O

P<sub>2</sub>/c C<sub>2h</sub><sup>5</sup> No. 14 (continued)

## Inorganic (continued)

0.9567	(Mg, Ca) <sub>2</sub> FP <sub>4</sub>	1.0219	Zr <sub>2</sub>
0.9575	PbCr <sub>4</sub>	1.0237	Hf <sub>2</sub>
0.9584	SrCr <sub>4</sub>	1.0264	Bi <sub>2</sub> Rh
0.9607	Bi <sub>2</sub> Mo <sub>3</sub> <sub>12</sub>	1.0290	As <sub>2</sub> Co
0.9609	PbCr <sub>4</sub>	1.0300	Ta <sub>2</sub> N
0.9657	(La, Ce, Y)P <sub>4</sub>	1.0399	HgSe <sub>4</sub> •H <sub>2</sub> <sub>g</sub>
0.9658	CeP <sub>4</sub>	1.0400	KCr <sub>3</sub> Cl
0.9662	PbSe <sub>4</sub>	1.0419	(Fe, Mn)Si <sub>3</sub>
0.9676	(Cu, Zn) <sub>3</sub> (OH) <sub>3</sub> P <sub>4</sub> •2H <sub>2</sub> <sub>g</sub>	1.0473	H <sub>6</sub> Te <sub>6</sub>
0.9680	CuK(CN) <sub>2</sub>	1.0492	KCr <sub>3</sub> Cl
0.9685	(La, Ce, Y)P <sub>4</sub>	1.0493	Na <sub>2</sub> S <sub>2</sub> <sub>3</sub>
0.9686	SrSe <sub>4</sub>	1.0528	K <sub>6</sub> V <sub>10</sub> <sub>28</sub> •10H <sub>2</sub> <sub>g</sub>
0.9688	LaP <sub>4</sub>	1.0575	ICl
0.9697	W <sub>3</sub>	1.0578	(Ca <sub>0.16</sub> Mg <sub>0.45</sub> Fe <sub>0.39</sub> )Si <sub>3</sub>
0.9697	NdP <sub>4</sub>	1.0583	Ca <sub>0.10</sub> Fe <sub>0.56</sub> Mg <sub>0.34</sub> Si <sub>3</sub>
0.9697	CmP <sub>4</sub>	1.0616	Na <sub>3</sub> PS <sub>4</sub> •8H <sub>2</sub> <sub>g</sub>
0.9698	(La, Ce, Y)P <sub>4</sub>	1.0629	MgNa <sub>6</sub> (S <sub>4</sub> ) <sub>4</sub>
0.9707	(Re, Th, Ca, U)(P, Si) <sub>4</sub>	1.0633	MgSi <sub>3</sub>
0.9722	NdAs <sub>4</sub>	1.0646	(Na, Ca) <sub>2</sub> (Fe, Mn)(Zr, Ti)(F, OH)Si <sub>2</sub> <sub>7</sub>
0.9723	SmP <sub>4</sub>	1.0656	Ni <sub>3</sub> (As <sub>4</sub> ) <sub>2</sub>
0.9723	CeAs <sub>4</sub>	1.0667	Al <sub>2</sub> Fe(OH) <sub>2</sub> (P <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> <sub>g</sub>
0.9727	PrP <sub>4</sub>	1.0676	Ca <sub>3</sub> Si <sub>2</sub> <sub>7</sub>
0.9733	PrAs <sub>4</sub>	1.0681	Ni <sub>2</sub> P <sub>2</sub> <sub>7</sub>
0.9739	(NH <sub>4</sub> ) <sub>2</sub> S <sub>2</sub> <sub>8</sub>	1.0684	CaNaB <sub>5</sub> <sub>9</sub> •5H <sub>2</sub> <sub>g</sub>
0.9740	NdP <sub>4</sub>	1.0695	(NH <sub>4</sub> ) <sub>10</sub> W <sub>12</sub> <sub>41</sub> •5H <sub>2</sub> <sub>g</sub>
0.9740	BiP <sub>4</sub>	1.0740	Cu <sub>2</sub> S <sub>3</sub> •CuS <sub>3</sub> •2H <sub>2</sub> <sub>g</sub>
0.9745	XeF <sub>4</sub>	1.0750	Mg <sub>2</sub> P <sub>2</sub> <sub>7</sub>
0.9753	PmP <sub>4</sub>	1.0765	Hg <sub>2</sub> <sub>g</sub> (N <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> <sub>g</sub>
0.9760	Cs <sub>2</sub> S <sub>2</sub> <sub>8</sub>	1.0776	C <sub>2</sub> B <sub>10</sub> <sub>16</sub>
0.9761	Mn <sub>2</sub> H <sub>2</sub> <sub>5</sub>	1.0829	TlAs <sub>2</sub>
0.9763	Ca <sub>2</sub> NaFSi <sub>4</sub>	1.0894	Na <sub>2</sub> Cr <sub>4</sub> •4H <sub>2</sub> <sub>g</sub>
0.9768	Al <sub>2</sub> Fe(OH) <sub>2</sub> (P <sub>4</sub> ) <sub>2</sub>	1.0902	ZnCl <sub>2</sub>
0.9769	PaSi <sub>4</sub>	1.0922	LiNa(BeF <sub>3</sub> ) <sub>2</sub>
0.9770	ThSi <sub>4</sub>	1.0947	NH <sub>4</sub> BiF <sub>4</sub>
0.9780	XeF <sub>4</sub>	1.1101	Al <sub>3</sub> Na(OH) <sub>4</sub> (P <sub>4</sub> ) <sub>2</sub>
0.9781	Al <sub>2</sub> (Fe, Mg)(OH) <sub>2</sub> (P <sub>4</sub> ) <sub>2</sub>	1.1108	[(Ce, Ca, La, Th)P <sub>4</sub> ]
0.9821	Al <sub>2</sub> (Mg <sub>0.8</sub> Fe <sub>0.2</sub> )(OH) <sub>2</sub> (P <sub>4</sub> ) <sub>2</sub>	1.1376	W <sub>2</sub>
0.9834	Al <sub>2</sub> Mg(OH) <sub>2</sub> (P <sub>4</sub> ) <sub>2</sub>	1.1389	Ag <sub>2</sub> S
0.9853	FeFe <sub>2</sub> (OH) <sub>2</sub> (P <sub>4</sub> ) <sub>2</sub>	1.1400	(S <sub>4</sub> N <sub>3</sub> )N <sub>3</sub>
0.9862	Al <sub>2</sub> (Mg, Fe)(OH) <sub>2</sub> (P <sub>4</sub> ) <sub>2</sub>	1.1465	K <sub>2</sub> Pd(CN) <sub>4</sub> •H <sub>2</sub> <sub>g</sub>
0.9891	Na <sub>2</sub> Zn <sub>2</sub> <sub>3</sub>	1.1489	Hg <sub>2</sub> <sub>g</sub> (N <sub>3</sub> ) <sub>2</sub> •2H <sub>2</sub> <sub>g</sub>
0.9916	(N <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> S <sub>4</sub>	1.1516	(S <sub>4</sub> N <sub>3</sub> )N <sub>3</sub>
0.9918	(H <sub>2</sub> N) <sub>3</sub> PBR <sub>3</sub>	1.1518	(NH <sub>4</sub> ) <sub>2</sub> S <sub>4</sub> <sub>6</sub>
0.9924	FeK(S <sub>4</sub> ) <sub>2</sub> •4H <sub>2</sub> <sub>g</sub>	1.1532	Mo <sub>2</sub>
0.9985	Hg <sub>3</sub> <sub>2</sub> Cl <sub>2</sub>	1.1548	FeCl <sub>2</sub> •4H <sub>2</sub> <sub>g</sub>
1.0000	AsCoS	1.1571	(S <sub>4</sub> N <sub>3</sub> )N <sub>3</sub>
1.0030	CrF <sub>2</sub>	1.1644	MoU <sub>9</sub>
1.0040	LiY <sub>2</sub>	1.1665	KZnCl <sub>3</sub> •2H <sub>2</sub> <sub>g</sub>
1.0045	K <sub>2</sub> RuN <sub>3</sub> (OH)(N <sub>3</sub> ) <sub>4</sub>	1.1674	BF <sub>3</sub> •2H <sub>2</sub> <sub>g</sub>
1.0046	S <sub>2</sub> N <sub>3</sub> HBr <sub>4</sub>	1.1691	H <sub>2</sub> S <sub>4</sub> •H <sub>2</sub> <sub>g</sub>
1.0055	S <sub>8</sub>	1.1709	Co(NH <sub>3</sub> ) <sub>3</sub> (N <sub>3</sub> ) <sub>2</sub> Br
1.0057	Mn <sub>2</sub> (OH)	1.1759	MnCl <sub>2</sub> •4H <sub>2</sub> <sub>g</sub>
1.0065	LiHo <sub>2</sub>	1.1779	Th <sub>2</sub> OH(N <sub>3</sub> ) <sub>3</sub> •4H <sub>2</sub> <sub>g</sub>
1.0094	Cs <sub>2</sub> U <sub>2</sub> Br <sub>4</sub>	1.1847	Cs <sub>4</sub> [Th(NCS) <sub>8</sub> ] <sub>2</sub> •2H <sub>2</sub> <sub>g</sub>
1.0100	NaMo <sub>2</sub> P <sub>4</sub>	1.1854	CaGa <sub>2</sub> <sub>4</sub>
1.0102	FeAsSe	1.1899	V <sub>2</sub>
1.0110	CuF <sub>2</sub>	1.1915	B <sub>5</sub> H <sub>11</sub>
1.0117	NaW <sub>2</sub> P <sub>4</sub>	1.1920	Co(N <sub>3</sub> ) <sub>2</sub> Br
1.0122	FePSe	1.1975	As <sub>2</sub> S <sub>3</sub>
1.0135	Hf <sub>2</sub>	1.1985	As <sub>2</sub> S <sub>3</sub>
1.0135	GaP <sub>4</sub> •2H <sub>2</sub> <sub>g</sub>	1.1996	MgH <sub>2</sub> <sub>3</sub>
1.0135	Fe <sub>2</sub> K(OH)(P <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> <sub>g</sub>	1.2083	As <sub>2</sub> Zn
1.0146	FeSbSe	1.2140	P <sub>2</sub> Zn
1.0152	FeSbS	1.2218	NH <sub>3</sub> OHCl
1.0175	AgF <sub>2</sub>	1.2221	S <sub>4</sub> N <sub>4</sub>
1.0180	FeAsTe	1.2360	Na <sub>2</sub> S <sub>4</sub> •10H <sub>2</sub> <sub>g</sub>
1.0196	Sc <sub>2</sub> F	1.2384	Na <sub>2</sub> (U <sub>2</sub> ) <sub>2</sub> V <sub>2</sub> <sub>8</sub>
1.0198	Zr <sub>2</sub>	1.2386	Na <sub>2</sub> S <sub>4</sub> •10H <sub>2</sub> <sub>g</sub>
1.0199	W <sub>3</sub>	1.2398	NH <sub>3</sub> OHBr
1.0202	FeSbTe	1.2412	KU <sub>2</sub> V <sub>4</sub>
1.0208	Zr <sub>2</sub>	1.2428	Ba <sub>2</sub> •H <sub>2</sub> <sub>g</sub> •2•2H <sub>2</sub> <sub>g</sub>
1.0211	LiDy <sub>2</sub>	1.2433	CsI <sub>4</sub>
1.0215	AgMo <sub>2</sub> P <sub>4</sub>	1.2438	Cs <sub>2</sub> (U <sub>2</sub> ) <sub>2</sub> V <sub>2</sub> <sub>8</sub>
1.0217	FePS	1.2444	Rb <sub>2</sub> (U <sub>2</sub> ) <sub>2</sub> V <sub>2</sub> <sub>8</sub>



P2<sub>1</sub>/c C<sub>2h</sub><sup>5</sup> No. 14 (continued)

## Inorganic (continued)

1.2444	Hg <sub>3</sub> P <sub>2</sub> I <sub>2</sub>	1.5554	MnTh(Nb <sub>3</sub> ) <sub>6</sub> •8H <sub>2</sub> O
1.2449	K <sub>2</sub> (UO <sub>2</sub> ) <sub>2</sub> V <sub>2</sub> O <sub>8</sub>	1.5559	NiTh(Nb <sub>3</sub> ) <sub>6</sub> •8H <sub>2</sub> O
1.2458	Ru <sub>4</sub> F <sub>20</sub>	1.5563	KSeCN
1.2461	Tl <sub>2</sub> (UO <sub>2</sub> ) <sub>2</sub> V <sub>2</sub> O <sub>8</sub>	1.5577	ThZn(Nb <sub>3</sub> ) <sub>6</sub> •8H <sub>2</sub> O
1.2476	Na <sub>2</sub> S <sub>6</sub> •10H <sub>2</sub> O	1.5654	CuP <sub>2</sub>
1.2632	Ca <sub>4</sub> B <sub>4</sub> (B <sub>6</sub> ) <sub>3</sub> (Si <sub>6</sub> ) <sub>3</sub> •H <sub>2</sub> O	1.5759	Rb <sub>2</sub> UO <sub>2</sub> (Nb <sub>3</sub> ) <sub>4</sub>
1.2647	CaBSi <sub>4</sub> (OH)	1.5846	Se
1.2667	Hg <sub>5</sub> Cl <sub>2</sub>	1.5866	BaB <sub>4</sub> O <sub>7</sub>
1.2672	V(OH) <sub>2</sub> S <sub>6</sub> •4H <sub>2</sub> O	1.5875	Rb <sub>2</sub> Pd(Nb <sub>2</sub> ) <sub>4</sub>
1.2709	V <sub>6</sub> S <sub>6</sub> •5H <sub>2</sub> O	1.5923	Se
1.2760	Ca(F,OH)BeP <sub>6</sub>	1.5960	LiAl <sub>4</sub> Si <sub>3</sub> Al <sub>10</sub> (OH) <sub>8</sub>
1.2774	Ca <sub>2</sub> FeB <sub>2</sub> O <sub>2</sub> (Si <sub>6</sub> ) <sub>2</sub>	1.6048	(NH <sub>4</sub> ) <sub>2</sub> HP <sub>6</sub>
1.2783	Ag <sub>4</sub> MnSb <sub>2</sub> S <sub>6</sub>	1.6121	Zn <sub>2</sub> (OH)As <sub>6</sub> •H <sub>2</sub> O
1.2786	Se <sub>8</sub>	1.6139	C <sub>6</sub> Pd(Nb <sub>2</sub> ) <sub>4</sub>
1.2791	Ba(OH) <sub>2</sub> •8H <sub>2</sub> O	1.6354	Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> •4H <sub>2</sub> O
1.2800	Se <sub>8</sub>	1.6354	C <sub>6</sub> P <sub>6</sub> O <sub>12</sub> •H <sub>2</sub> O
1.2889	Rb <sub>3</sub> Fe(CN) <sub>6</sub>	1.6381	ThI <sub>4</sub>
1.2931	HAuCl <sub>4</sub> •4H <sub>2</sub> O	1.6472	Na <sub>2</sub> B <sub>4</sub> O <sub>6</sub> (OH) <sub>2</sub> •3H <sub>2</sub> O
1.2969	(NH <sub>4</sub> ) <sub>3</sub> Se <sub>4</sub> Nb <sub>3</sub>	1.6540	N <sub>2</sub> O <sub>2</sub>
1.2992	AsSbS <sub>3</sub>	1.6753	SrB <sub>6</sub> O <sub>6</sub> (OH) <sub>2</sub> •3H <sub>2</sub> O
1.2992	SnCl <sub>2</sub> •2H <sub>2</sub> O	1.6778	SrB <sub>6</sub> O <sub>10</sub> •4H <sub>2</sub> O
1.3108	FeY <sub>2</sub> (BeSi <sub>5</sub> ) <sub>2</sub>	1.6870	Na <sub>2</sub> Str <sub>2</sub> Al <sub>2</sub> (F <sub>6</sub> ) <sub>4</sub> F <sub>9</sub>
1.3111	Cu(UO <sub>2</sub> ) <sub>2</sub> (V <sub>6</sub> ) <sub>2</sub> •8-10H <sub>2</sub> O	1.6966	K <sub>2</sub> Ni(CN) <sub>4</sub>
1.3152	FeY <sub>2</sub> (BeSi <sub>5</sub> ) <sub>2</sub>	1.7003	B <sub>9</sub> H <sub>15</sub>
1.3266	Cu <sub>4</sub> (OH) <sub>6</sub> S <sub>6</sub>	1.7051	Li <sub>2</sub> S <sub>6</sub>
1.3312	N <sub>2</sub> H <sub>6</sub> (H <sub>2</sub> P <sub>6</sub> ) <sub>2</sub>	1.7112	RbSb <sub>2</sub> Cl <sub>7</sub> •H <sub>2</sub> O
1.3317	Pt(NH <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	1.7376	Mg <sub>2</sub> UO <sub>2</sub> (C <sub>6</sub> ) <sub>3</sub> •18H <sub>2</sub> O
1.3350	Pt(NH <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	1.7396	BaFeMn <sub>7</sub> O <sub>16</sub>
1.3426	Na <sub>2</sub> Zn(S <sub>6</sub> ) <sub>2</sub> •4H <sub>2</sub> O	1.7407	Mg <sub>2</sub> UO <sub>2</sub> (C <sub>6</sub> ) <sub>3</sub> •18H <sub>2</sub> O
1.3516	KOH•H <sub>2</sub> O	1.7429	(NH <sub>4</sub> ) <sub>4</sub> UF <sub>8</sub>
1.3532	Pd(NS <sub>3</sub> ) <sub>2</sub>	1.7491	Ba(B <sub>6</sub> ) <sub>2</sub> •5H <sub>2</sub> O
1.3546	MgNa <sub>2</sub> (S <sub>6</sub> ) <sub>2</sub> •4H <sub>2</sub> O	1.7524	NaSb
1.3603	Al <sub>9</sub> Co <sub>2</sub>	1.7548	C <sub>2</sub> Ca
1.3623	Fe <sub>2</sub> (S <sub>6</sub> ) <sub>3</sub>	1.7563	RbBi <sub>2</sub> Cl <sub>7</sub> •H <sub>2</sub> O
1.3636	Ba <sub>2</sub> Ti <sub>6</sub>	1.7583	Na <sub>2</sub> S <sub>6</sub> •7H <sub>2</sub> O
1.3690	N <sub>2</sub> O <sub>4</sub>	1.7692	Cu <sub>3</sub> (OH) <sub>2</sub> (C <sub>6</sub> ) <sub>2</sub>
1.3728	Ca <sub>2</sub> Si <sub>6</sub>	1.7756	CaB <sub>6</sub> O <sub>10</sub> •4H <sub>2</sub> O
1.3778	Na <sub>2</sub> BeF <sub>4</sub>	1.7791	GeNa
1.3797	Zr(S <sub>6</sub> ) <sub>2</sub> •1.5H <sub>2</sub> O	1.7828	[(NH <sub>3</sub> ) <sub>5</sub> Co <sub>6</sub> ] <sub>2</sub> HS <sub>6</sub> (S <sub>6</sub> ) <sub>2</sub> •2H <sub>2</sub> O
1.3812	CsH <sub>5</sub> (As <sub>6</sub> ) <sub>2</sub>	1.7874	Rb <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>
1.3842	FeNa <sub>2</sub> (S <sub>6</sub> ) <sub>2</sub> •4H <sub>2</sub> O	1.7886	K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>
1.3844	Ca <sub>2</sub> (OH) <sub>5</sub> H <sub>5</sub> Si <sub>6</sub>	1.7937	Fe <sub>6</sub> Cr <sub>6</sub>
1.3904	Na <sub>3</sub> AlF <sub>6</sub>	1.7992	Pb <sub>2</sub> V <sub>2</sub> O <sub>7</sub>
1.3904	Na <sub>3</sub> AlH <sub>6</sub>	1.8056	NH <sub>4</sub> CNS
1.3976	Na <sub>3</sub> ScF <sub>6</sub>	1.8074	BeNaP <sub>6</sub>
1.4018	CsH <sub>5</sub> (P <sub>6</sub> ) <sub>2</sub>	1.8147	Ag <sub>2</sub> Te
1.4121	Hg <sub>2</sub> SbBr <sub>2</sub>	1.8206	AsLi
1.4167	K <sub>2</sub> TeBr <sub>6</sub>	1.8240	Pb <sub>2</sub> (Cl <sub>6</sub> ) <sub>2</sub> •2H <sub>2</sub> O
1.4347	Ca <sub>3</sub> (P <sub>6</sub> ) <sub>2</sub>	1.8436	Co(Nb) <sub>2</sub> Cl
1.4374	Cr(Nb <sub>3</sub> ) <sub>3</sub> •9H <sub>2</sub> O	1.8529	Pb <sub>2</sub> V <sub>2</sub> O <sub>7</sub>
1.4386	Al <sub>2</sub> Br <sub>6</sub>	1.8575	Pb <sub>2</sub> V <sub>2</sub> O <sub>7</sub>
1.4421	Al(Nb <sub>3</sub> ) <sub>3</sub> •9H <sub>2</sub> O	1.8622	(Mn,Fe) <sub>2</sub> (OH)P <sub>6</sub>
1.4486	Pt(SN) <sub>4</sub>	1.8746	Mn <sub>2</sub> (OH)As <sub>6</sub>
1.4489	Ca <sub>5</sub> Si <sub>2</sub> O <sub>7</sub> (C <sub>6</sub> ) <sub>2</sub>	1.8801	CaAl <sub>2</sub> O <sub>4</sub>
1.4663	Bi <sub>8</sub> O <sub>5</sub> (OH) <sub>5</sub> (As <sub>6</sub> ) <sub>3</sub>	1.8887	NaP <sub>6</sub>
1.4683	TiBr <sub>4</sub>	1.8929	HNb <sub>3</sub>
1.4759	CdP <sub>4</sub>	1.9013	Rb <sub>2</sub> Th(Nb <sub>3</sub> ) <sub>6</sub>
1.4762	KCu <sub>2</sub> (CN) <sub>3</sub> •H <sub>2</sub> O	1.9174	Al(OH) <sub>3</sub>
1.4785	SnCl <sub>4</sub>	1.9181	KAuCl <sub>4</sub>
1.4832	LiB <sub>6</sub>	1.9206	Cu <sub>3</sub> (OH) <sub>3</sub> As <sub>6</sub>
1.4841	KCu <sub>2</sub> (CN) <sub>3</sub> •H <sub>2</sub> O	1.9259	Cu <sub>3</sub> (OH) <sub>3</sub> As <sub>6</sub>
1.4846	HI <sub>3</sub> O <sub>8</sub>	1.9375	Fe(OH) <sub>3</sub>
1.5014	SnBr <sub>4</sub>	1.9422	K <sub>3</sub> Co(CN) <sub>6</sub>
1.5046	TiCl <sub>4</sub>	1.9517	NaP <sub>6</sub>
1.5057	LiB <sub>6</sub>	1.9548	NaP <sub>6</sub>
1.5065	S <sub>2</sub> PN <sub>3</sub> O <sub>2</sub> Cl <sub>4</sub>	1.9570	PbUTE <sub>2</sub> O <sub>8</sub>
1.5092	TiCl <sub>4</sub>	1.9574	AgP <sub>6</sub>
1.5272	NH <sub>4</sub> B <sub>5</sub> O <sub>8</sub> •2H <sub>2</sub> O	1.9779	Cr(NH <sub>3</sub> ) <sub>3</sub> O <sub>4</sub>
1.5310	(NH <sub>4</sub> ) <sub>5</sub> [Ir(S <sub>6</sub> ) <sub>2</sub> Cl <sub>4</sub> ]	1.9841	Z(UO <sub>2</sub> ) <sub>2</sub> Cr <sub>6</sub> •UO <sub>3</sub> •4H <sub>2</sub> O
1.5334	(NH <sub>4</sub> ) <sub>2</sub> S <sub>6</sub> O <sub>3</sub> •H <sub>2</sub> O	1.9980	Na <sub>2</sub> SnF <sub>6</sub>
1.5435	AgF <sub>2</sub>	1.9985	In <sub>2</sub> I <sub>6</sub>
1.5507	NaSbF <sub>4</sub>	2.0087	CuSb <sub>2</sub> O <sub>6</sub>
1.5513	CoTh(Nb <sub>3</sub> ) <sub>6</sub> •8H <sub>2</sub> O	2.0159	BaS <sub>4</sub> O <sub>6</sub> •2H <sub>2</sub> O
1.5554	MgTh(Nb <sub>3</sub> ) <sub>6</sub> •8H <sub>2</sub> O	2.0195	Ag <sub>2</sub> B <sub>8</sub> O <sub>13</sub>

P2<sub>1</sub>/c C<sub>2h</sub><sup>5</sup> No. 14 (continued)

## Inorganic (continued)

2.0315	(Fe, Mn)Zn <sub>2</sub> (P <sub>4</sub> ) <sub>2</sub> •4H <sub>2</sub> O	2.5100	K <sub>2</sub> Se(S <sub>6</sub> ) <sub>2</sub>
2.0423	(Ag <sub>7</sub> Te)(N <sub>3</sub> ) <sub>5</sub>	2.5380	Na <sub>2</sub> Si <sub>2</sub> O <sub>5</sub>
2.0694	KTeO(OH) <sub>5</sub> •H <sub>2</sub> O	2.5517	(NH <sub>4</sub> ) <sub>2</sub> H <sub>10</sub> H <sub>10</sub> •xH <sub>2</sub> O
2.0733	Na <sub>3</sub> PS <sub>4</sub> •8H <sub>2</sub> O	2.6096	KBCl <sub>3</sub>
2.0737	Pb <sub>3</sub> (OH) <sub>2</sub> Cl <sub>4</sub>	2.6140	PbWO <sub>4</sub>
2.0830	CaSiO <sub>3</sub>	2.6164	Sb <sub>4</sub> O <sub>5</sub> Br <sub>2</sub>
2.1040	Ca <sub>2</sub> UO <sub>5</sub>	2.6434	Sb <sub>4</sub> O <sub>5</sub> Cl <sub>2</sub>
2.1058	CaSiO <sub>3</sub>	2.6654	Li <sub>6</sub> Ge <sub>2</sub> O <sub>7</sub>
2.1075	Sr <sub>2</sub> UO <sub>5</sub>	2.6869	LaTaO <sub>4</sub>
2.1093	CaSiO <sub>3</sub>	2.7225	Cu(SCN) <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub> •Cu(SCN)(NH <sub>3</sub> )
2.1094	NbI <sub>5</sub>	2.7327	PrTaO <sub>4</sub>
2.1119	Ca <sub>5</sub> (SiO <sub>4</sub> ) <sub>2</sub> CO <sub>3</sub>	2.7354	Na <sub>2</sub> N <sub>2</sub> O <sub>2</sub> •5H <sub>2</sub> O
2.1183	CdSiO <sub>3</sub>	2.8071	(Pb, Cu, Fe) <sub>3</sub> [(Cr, As, P) <sub>4</sub> ] <sub>2</sub> (OH)
2.1257	NaBeF <sub>3</sub>	2.8123	(NH <sub>4</sub> ) <sub>2</sub> UO <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> O
2.1433	Ce(FeO <sub>4</sub> ) <sub>3</sub> •4H <sub>2</sub> O	2.8219	ICl
2.1523	Mn <sub>5</sub> (OH) <sub>2</sub> (SiO <sub>4</sub> ) <sub>2</sub>	2.8333	(NH <sub>4</sub> ) <sub>6</sub> Mo <sub>7</sub> O <sub>26</sub> •6H <sub>2</sub> O
2.1559	H <sub>3</sub> N•B <sub>3</sub> H <sub>7</sub>	2.8673	RbPO <sub>3</sub>
2.1573	CoSO <sub>4</sub> •7H <sub>2</sub> O	2.8830	Mg <sub>9</sub> (OH, F) <sub>2</sub> (SiO <sub>4</sub> ) <sub>4</sub>
2.1590	(Fe, Cu, Zn)SO <sub>4</sub> •7H <sub>2</sub> O	2.8954	K <sub>2</sub> MoO <sub>2</sub> (F) <sub>4</sub> •R <sub>2</sub> O
2.1639	FeSO <sub>4</sub> •7H <sub>2</sub> O	2.9197	K <sub>2</sub> MoO <sub>2</sub> F <sub>4</sub> •H <sub>2</sub> O
2.1670	Na <sub>3</sub> (NHP <sub>2</sub> ) <sub>3</sub> •4H <sub>2</sub> O	2.9273	AlCaNaF <sub>6</sub> •H <sub>2</sub> O
2.1699	Mg <sub>5</sub> (OH, F) <sub>2</sub> (SiO <sub>4</sub> ) <sub>2</sub>	2.9289	Mn <sub>9</sub> Si <sub>4</sub> O <sub>16</sub> (OH, F) <sub>2</sub>
2.1725	(NH <sub>4</sub> ) <sub>2</sub> As <sub>2</sub> F <sub>8</sub> O <sub>2</sub>	2.9421	CaPO <sub>3</sub>
2.1731	Pb(P <sub>2</sub> O <sub>5</sub> ) <sub>2</sub>	2.9618	Cu <sub>5</sub> (OH) <sub>4</sub> (P <sub>2</sub> O <sub>5</sub> ) <sub>2</sub>
2.1763	(Fe, Mn, Ca) <sub>3</sub> (P <sub>2</sub> O <sub>5</sub> ) <sub>2</sub>	2.9680	Ba <sub>2</sub> Si <sub>3</sub> O <sub>8</sub>
2.1812	(Fe, Mn, Mg) <sub>3</sub> (P <sub>2</sub> O <sub>5</sub> ) <sub>2</sub>	2.9704	Cu <sub>5</sub> (OH) <sub>4</sub> (P <sub>2</sub> O <sub>5</sub> ) <sub>2</sub>
2.2124	MnZn <sub>2</sub> (OH) <sub>2</sub> SiO <sub>4</sub>	3.0036	K <sub>2</sub> Te(S <sub>2</sub> O <sub>3</sub> ) <sub>2</sub>
2.2128	Ca(P <sub>2</sub> O <sub>5</sub> ) <sub>2</sub>	3.0286	Ag <sub>3</sub> Pb <sub>2</sub> Sb <sub>3</sub> S <sub>8</sub>
2.2150	Sr <sub>2</sub> B <sub>2</sub> O <sub>5</sub>	3.0310	Cu <sub>5</sub> (OH) <sub>4</sub> (AsO <sub>4</sub> ) <sub>2</sub>
2.2263	MgCO <sub>3</sub> •3H <sub>2</sub> O	3.0881	KPO <sub>3</sub>
2.2277	Ca <sub>5</sub> H <sub>2</sub> (AsO <sub>4</sub> ) <sub>4</sub> •5H <sub>2</sub> O	3.1090	RbHSO <sub>4</sub>
2.2473	Fe <sub>3</sub> (P <sub>2</sub> O <sub>5</sub> ) <sub>2</sub> •4H <sub>2</sub> O	3.1549	(Pb, Tl) <sub>3</sub> As <sub>4</sub> (As, Ag) <sub>5</sub> S <sub>10</sub>
2.2614	Ca <sub>5</sub> (OH) <sub>2</sub> (SiO <sub>4</sub> ) <sub>2</sub>	3.1606	Pb <sub>7</sub> As <sub>9</sub> S <sub>20</sub>
2.2635	Fe <sub>3</sub> (P <sub>2</sub> O <sub>5</sub> ) <sub>2</sub> •4H <sub>2</sub> O	3.1674	LiAl <sub>4</sub> (OH) <sub>8</sub> Si <sub>3</sub> Al <sub>6</sub> O <sub>10</sub>
2.2820	NaPO <sub>3</sub>	3.1732	Pb <sub>13</sub> As <sub>18</sub> S <sub>40</sub>
2.2833	SO <sub>3</sub>	3.8782	Mg <sub>2</sub> B <sub>2</sub> O <sub>5</sub>
2.2865	Ca <sub>2</sub> SiO <sub>4</sub> •H <sub>2</sub> O	3.8854	(Cu, Zn) <sub>3</sub> (OH) <sub>4</sub> SO <sub>4</sub> •2H <sub>2</sub> O
2.3208	K <sub>2</sub> As <sub>2</sub> F <sub>8</sub> O <sub>2</sub>	4.0000	BaTe(S <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> •3H <sub>2</sub> O
2.3311	Rb <sub>2</sub> As <sub>2</sub> F <sub>8</sub> O <sub>2</sub>	4.1690	(HBS <sub>2</sub> ) <sub>3</sub>
2.3314	(NH <sub>4</sub> ) <sub>2</sub> [Ru(N <sub>3</sub> )(OH)Cl <sub>4</sub> ]	4.1699	Br <sub>3</sub> B <sub>3</sub> S <sub>3</sub>
2.3465	CuPb <sub>2</sub> (CrO <sub>4</sub> )(P <sub>2</sub> O <sub>5</sub> )	4.5116	K <sub>3</sub> Co(CN) <sub>6</sub>
2.3750	H <sub>3</sub> P <sub>2</sub> O <sub>4</sub>	4.5119	Mo <sub>4</sub> O <sub>11</sub>
2.4000	Pb <sub>2</sub> P <sub>2</sub> S <sub>5</sub>	4.5347	Na <sub>2</sub> P <sub>4</sub> O <sub>11</sub>
2.4049	H <sub>3</sub> P <sub>2</sub> O <sub>4</sub>	5.1633	K <sub>2</sub> S <sub>2</sub> O <sub>3</sub> •0.33H <sub>2</sub> O
2.4120	Pb <sub>2</sub> Si <sub>4</sub>	5.4271	HgSb <sub>4</sub> S <sub>7</sub>
2.4754	UO <sub>2</sub> WO <sub>4</sub>	6.3687	PdBr <sub>2</sub>
2.4799	UO <sub>2</sub> MoO <sub>4</sub>	6.5261	C <sub>24</sub> H <sub>50</sub>
2.4867	PbAs <sub>2</sub> S <sub>4</sub>	7.4651	PbAs <sub>2</sub> S <sub>4</sub>

## Organic

0.1101	Sr(C <sub>12</sub> H <sub>23</sub> O <sub>2</sub> ) <sub>2</sub>	0.3063	C <sub>16</sub> H <sub>18</sub> N <sub>3</sub> SeBr•5H <sub>2</sub> O
0.1805	BrNH <sub>3</sub> C <sub>6</sub> H <sub>10</sub> COOH	0.3079	C <sub>16</sub> H <sub>18</sub> N <sub>3</sub> SBr•5H <sub>2</sub> O
0.1953	CH <sub>3</sub> CO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> •C <sub>6</sub> H <sub>4</sub> Cl	0.3086	CN(CH <sub>2</sub> ) <sub>2</sub> CN•2AgNO <sub>3</sub>
0.1974	C <sub>6</sub> H <sub>5</sub> NHNH <sub>2</sub> •HCl	0.3096	C <sub>16</sub> H <sub>18</sub> N <sub>3</sub> SCL•5H <sub>2</sub> O
0.2125	ClC <sub>6</sub> H <sub>4</sub> •C <sub>6</sub> H <sub>4</sub> COOH	0.3152	(NH <sub>2</sub> •C•CN) <sub>2</sub>
0.2181	C <sub>5</sub> H <sub>9</sub> N <sub>2</sub> O <sub>2</sub> •H <sub>2</sub> O	0.3169	C <sub>2</sub> H <sub>2</sub> N <sub>2</sub>
0.2259	(C <sub>7</sub> H <sub>5</sub> CLNO <sub>2</sub> ) <sub>2</sub> Pd	0.3237	[(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> ] <sub>3</sub> As
0.2265	FC <sub>6</sub> H <sub>4</sub> •C <sub>6</sub> H <sub>4</sub> COOH	0.3242	Ir(CO)((C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> PCH <sub>2</sub> CH <sub>2</sub> P(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ) <sub>2</sub> Cl
0.2273	(C <sub>7</sub> H <sub>5</sub> CLNO <sub>2</sub> ) <sub>2</sub> Ni	0.3250	C <sub>15</sub> H <sub>12</sub> O <sub>5</sub>
0.2281	C <sub>11</sub> H <sub>17</sub> NO•HBr	0.3278	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>
0.2390	Pt(C <sub>7</sub> H <sub>5</sub> O <sub>2</sub> N) <sub>2</sub>	0.3341	C <sub>2</sub> H <sub>9</sub> B <sub>10</sub> I <sub>3</sub>
0.2472	(CH <sub>2</sub> CO) <sub>2</sub>	0.3395	HgCl <sub>2</sub> •C <sub>5</sub> H <sub>3</sub> Br <sub>2</sub> N <sub>6</sub>
0.2491	ONC <sub>6</sub> H <sub>4</sub> OH	0.3427	C <sub>10</sub> H <sub>26</sub> N <sub>4</sub> •2H <sub>3</sub> PO <sub>4</sub> •6H <sub>2</sub> O
0.2556	C <sub>40</sub> H <sub>54</sub>	0.3439	C <sub>6</sub> H <sub>10</sub> (OH) <sub>2</sub>
0.2654	CCl <sub>2</sub> :C(C <sub>6</sub> H <sub>4</sub> Cl) <sub>2</sub>	0.3563	(PhCl(C <sub>8</sub> H <sub>12</sub> )) <sub>2</sub>
0.2740	(NO <sub>2</sub> •NNA•CH <sub>2</sub> ) <sub>2</sub>	0.3581	C <sub>15</sub> H <sub>26</sub> Cl <sub>2</sub>
0.2785	Te(C <sub>8</sub> H <sub>17</sub> S) <sub>4</sub> (N <sub>3</sub> ) <sub>2</sub>	0.3599	C <sub>8</sub> H <sub>6</sub> CLNO <sub>3</sub>
0.2824	NH <sub>2</sub> CH <sub>2</sub> COOH•AgNO <sub>3</sub>	0.3625	C <sub>9</sub> H <sub>16</sub> O <sub>4</sub>
0.2875	C <sub>8</sub> H <sub>7</sub> BrO <sub>2</sub>	0.3633	C <sub>6</sub> H <sub>5</sub> •CH(C <sub>2</sub> H <sub>5</sub> )•CH(C <sub>2</sub> H <sub>5</sub> )•C <sub>6</sub> H <sub>5</sub>
0.2921	C <sub>5</sub> H <sub>6</sub> O <sub>3</sub>	0.3646	C <sub>7</sub> H <sub>14</sub> N <sub>10</sub> O <sub>8</sub>
0.2947	CH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> •CH <sub>2</sub> •CH•COOH	0.3653	C <sub>28</sub> H <sub>14</sub> (CH <sub>3</sub> ) <sub>2</sub> O <sub>2</sub>
0.2953	CH <sub>3</sub> ZnSC <sub>4</sub> H <sub>9</sub>	0.3683	C <sub>8</sub> H <sub>15</sub> N <sub>6</sub> •HBr
0.3030	NH <sub>4</sub> Ag(SCN) <sub>2</sub>	0.3709	C <sub>17</sub> H <sub>19</sub> CLN <sub>2</sub> •SHCl
0.3039	C <sub>16</sub> H <sub>18</sub> N <sub>3</sub> SCL•4H <sub>2</sub> O	0.3709	C <sub>2</sub> H <sub>4</sub> I <sub>2</sub>

P2<sub>1</sub>/c C<sub>2h</sub><sup>5</sup> No. 14 (continued)

## Organic (continued)

0.3714	C <sub>28</sub> H <sub>14</sub> Br <sub>2</sub> θ <sub>2</sub>	0.4965	Mn(C <sub>7</sub> H <sub>4</sub> Nθ <sub>3</sub> S) <sub>2</sub>
0.3721	NH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> Sθ <sub>3</sub> •H <sub>2</sub> θ	0.4979	[(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> N <sub>2</sub> Cl]CuCl <sub>2</sub>
0.3797	C <sub>4</sub> S <sub>2</sub> (CN) <sub>4</sub>	0.4980	Ni(C <sub>7</sub> H <sub>4</sub> Nθ <sub>3</sub> S) <sub>2</sub>
0.3801	[(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> As] <sub>2</sub> θ	0.5005	C <sub>23</sub> H <sub>16</sub> N <sub>2</sub> θ
0.3815	C <sub>28</sub> H <sub>22</sub>	0.5011	[(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> P] <sub>2</sub> (CS)RhCl
0.3820	CH <sub>3</sub> θ•C <sub>6</sub> H <sub>4</sub> •C(C <sub>2</sub> H <sub>5</sub> ):C(C <sub>2</sub> H <sub>5</sub> )•C <sub>6</sub> H <sub>4</sub> θCH <sub>3</sub>	0.5022	Co(C <sub>5</sub> H <sub>4</sub> Nθ <sub>3</sub> S) <sub>2</sub>
0.3834	CH <sub>3</sub> •CH•C <sub>6</sub> H <sub>5</sub> •CH•C <sub>6</sub> H <sub>5</sub> •CH <sub>3</sub>	0.5030	(CHCθθH) <sub>2</sub>
0.3848	C <sub>16</sub> H <sub>6</sub> θ <sub>2</sub> S <sub>2</sub>	0.5046	Br <sub>2</sub> C <sub>6</sub> H <sub>3</sub> •N <sub>2</sub> •NH•C <sub>6</sub> H <sub>5</sub>
0.3851	CdCl <sub>2</sub> •2C <sub>2</sub> H <sub>5</sub> N <sub>3</sub> θ <sub>2</sub>	0.5075	HθθCCH:CHCθθH
0.3851	NaB <sub>10</sub> H <sub>13</sub> •2(CH <sub>3</sub> ) <sub>2</sub> θ	0.5087	C <sub>6</sub> H <sub>5</sub> SC <sub>6</sub> H <sub>4</sub> Nθ <sub>2</sub>
0.3885	C <sub>16</sub> H <sub>6</sub> θ <sub>2</sub> S <sub>2</sub> θ	0.5094	HθC <sub>6</sub> H <sub>4</sub> CHθ
0.3900	(C <sub>2</sub> H <sub>5</sub> )(C <sub>6</sub> H <sub>5</sub> )C <sub>5</sub> H <sub>2</sub> Nθ <sub>2</sub> Br	0.5130	CH <sub>3</sub> (CH <sub>3</sub> θ)Co(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> P•Cr(Cθ) <sub>4</sub>
0.3906	C <sub>8</sub> H <sub>6</sub> ClNθ <sub>3</sub>	0.5141	C <sub>9</sub> H <sub>7</sub> N•HCl
0.3948	C <sub>10</sub> H <sub>24</sub> N <sub>2</sub> Cl <sub>2</sub> •2H <sub>2</sub> θ	0.5153	(C <sub>6</sub> H <sub>4</sub> CθSθ <sub>2</sub> N) <sub>2</sub> Cu•6H <sub>2</sub> θ
0.3951	C <sub>13</sub> H <sub>14</sub> INθ <sub>2</sub>	0.5169	K <sub>3</sub> Fe(C <sub>2</sub> θ <sub>4</sub> ) <sub>3</sub> •3H <sub>2</sub> θ
0.3979	C <sub>6</sub> H <sub>6</sub> •CuAlCl <sub>4</sub>	0.5181	C <sub>6</sub> H <sub>4</sub> (CHθNθ <sub>2</sub> ) <sub>2</sub>
0.3989	K <sub>2</sub> C <sub>4</sub> H <sub>2</sub> θ <sub>4</sub> •2H <sub>2</sub> θ	0.5181	Te(C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> S) <sub>4</sub> Cl <sub>2</sub> •2H <sub>2</sub> θ
0.3990	C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> S	0.5195	C <sub>34</sub> H <sub>21</sub> Br <sub>2</sub> N <sub>7</sub> θ <sub>3</sub> S <sub>4</sub> •0.5C <sub>7</sub> H <sub>8</sub> θ
0.3994	(C <sub>5</sub> H <sub>8</sub> θ <sub>2</sub> N) <sub>2</sub> Cu•2H <sub>2</sub> θ	0.5210	Tl <sub>3</sub> Rh(C <sub>2</sub> θ <sub>4</sub> ) <sub>3</sub> •2H <sub>2</sub> θ
0.4002	Hrh(Cθ)[P(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> ] <sub>3</sub>	0.5227	(CH <sub>3</sub> Cθθ) <sub>2</sub>
0.4027	(CH <sub>3</sub> ) <sub>3</sub> N(CH <sub>2</sub> ) <sub>6</sub> N(CH <sub>3</sub> ) <sub>3</sub> •Br <sub>2</sub> •2H <sub>2</sub> θ	0.5229	[(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> Co(Nθ <sub>2</sub> )(NH <sub>2</sub> )Co(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> ](Nθ <sub>3</sub> ) <sub>4</sub>
0.4056	C <sub>8</sub> H <sub>18</sub> ClNθ•H <sub>2</sub> θ	0.5233	SeP(C <sub>6</sub> H <sub>4</sub> CR <sub>3</sub> ) <sub>3</sub>
0.4098	BrC <sub>6</sub> H <sub>4</sub> CH:CHCθθCH <sub>3</sub>	0.5246	C <sub>6</sub> H <sub>10</sub> S <sub>4</sub>
0.4112	C <sub>25</sub> H <sub>30</sub> Nθ <sub>3</sub> I	0.5260	SP(C <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> ) <sub>3</sub>
0.4114	CoCl <sub>2</sub> •(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> )(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	0.5268	K <sub>3</sub> [Cr(C <sub>2</sub> θ <sub>4</sub> ) <sub>3</sub> ]•3H <sub>2</sub> θ
0.4121	C <sub>4</sub> H <sub>4</sub> θ <sub>6</sub> •2H <sub>2</sub> θ	0.5274	K[Moθ <sub>2</sub> (C <sub>2</sub> θ <sub>4</sub> )•H <sub>2</sub> θ]
0.4125	C <sub>6</sub> H <sub>5</sub> Cl <sub>5</sub>	0.5281	(NH <sub>2</sub> CθNH <sub>3</sub> )CdCl <sub>3</sub>
0.4157	ClCH <sub>2</sub> CθθH	0.5282	C <sub>32</sub> H <sub>38</sub> N <sub>4</sub>
0.4266	NH <sub>2</sub> C <sub>6</sub> H <sub>10</sub> NH <sub>2</sub> •2HCl	0.5282	Cθ(C(Nθ <sub>2</sub> ) <sub>3</sub> )
0.4282	Hθ•C <sub>6</sub> H <sub>4</sub> •CH:CH•CθθH	0.5299	(CH <sub>3</sub> ) <sub>2</sub> C <sub>16</sub> H <sub>24</sub>
0.4311	C <sub>6</sub> H <sub>5</sub> CH:CHCθθH	0.5306	Rb <sub>3</sub> [Cr(C <sub>2</sub> θ <sub>4</sub> ) <sub>3</sub> ]•3H <sub>2</sub> θ
0.4326	[(C <sub>4</sub> H <sub>5</sub> ) <sub>3</sub> P] <sub>2</sub> Pd <sub>2</sub> Cl <sub>2</sub> C <sub>2</sub> θ <sub>4</sub>	0.5333	C <sub>6</sub> H <sub>8</sub> •2[θθ(Cθ) <sub>3</sub> ]
0.4349	(H <sub>2</sub> NC <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(C <sub>2</sub> H <sub>4</sub> NH <sub>2</sub> ) <sub>2</sub> •SHCl	0.5382	C <sub>6</sub> H <sub>6</sub> (θH) <sub>6</sub> •2H <sub>2</sub> θ
0.4386	HgCl <sub>2</sub> •3[(NH <sub>2</sub> ) <sub>2</sub> CS]	0.5385	Sθ(C <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> ) <sub>3</sub>
0.4475	NH <sub>2</sub> CθNHθCθNH <sub>2</sub> •0.79H <sub>2</sub> θ	0.5396	C <sub>8</sub> H <sub>8</sub> Nθ <sub>3</sub> Br
0.4485	CH <sub>3</sub> θ•C <sub>6</sub> H <sub>4</sub> •CH:CH•CθθH	0.5413	(CHθH) <sub>6</sub> •2H <sub>2</sub> θ
0.4488	(CH <sub>3</sub> •C(CH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> Ni	0.5468	AgCN•2AgNθ <sub>3</sub>
0.4521	NH <sub>2</sub> Cθ•NH•Cθ•NH <sub>2</sub> •0.6H <sub>2</sub> θ	0.5483	H•C(•S)•N(CH <sub>3</sub> )•CH <sub>2</sub> •C <sub>6</sub> H <sub>5</sub>
0.4525	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> θ <sub>2</sub>	0.5485	(CH <sub>3</sub> )(C <sub>6</sub> H <sub>5</sub> )(C <sub>2</sub> H <sub>5</sub> Cθθ)C <sub>5</sub> H <sub>8</sub> N•HBr
0.4536	Rb(C <sub>3</sub> H <sub>3</sub> θ <sub>3</sub> )H <sub>2</sub> θ	0.5491	(CH <sub>2</sub> -CH <sub>2</sub> CθθH) <sub>2</sub> (NH <sub>2</sub> (CH <sub>2</sub> ) <sub>3</sub> ) <sub>2</sub>
0.4559	NH <sub>2</sub> CH <sub>2</sub> CθθH	0.5496	(CH <sub>3</sub> )(C <sub>6</sub> H <sub>5</sub> )(C <sub>2</sub> H <sub>5</sub> Cθθ)C <sub>5</sub> H <sub>8</sub> N•HI
0.4560	AlCl <sub>3</sub> •C <sub>6</sub> H <sub>5</sub> Nθ <sub>2</sub>	0.5499	C <sub>8</sub> H <sub>8</sub> ClNθ <sub>3</sub>
0.4574	CH <sub>3</sub> Cθ•NH•CSe•NH•C <sub>6</sub> H <sub>5</sub>	0.5514	C <sub>10</sub> H <sub>6</sub> ClNθ <sub>2</sub>
0.4579	(C <sub>5</sub> H <sub>4</sub> •C <sub>5</sub> H <sub>4</sub> )Fe <sub>2</sub> (CH <sub>3</sub> Cθ•C <sub>5</sub> H <sub>4</sub> ) <sub>2</sub>	0.5522	Uθ <sub>2</sub> C <sub>2</sub> θ <sub>4</sub> •3H <sub>2</sub> θ
0.4600	C <sub>6</sub> H <sub>5</sub> Br <sub>2</sub> Nθ	0.5535	Ni(C <sub>13</sub> H <sub>18</sub> ClN <sub>2</sub> θ) <sub>2</sub>
0.4610	Fe(C <sub>5</sub> H <sub>4</sub> CθC <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.5546	(NH <sub>2</sub> CSNH <sub>2</sub> ) <sub>3</sub> Te(HF <sub>2</sub> ) <sub>2</sub>
0.4623	C <sub>6</sub> H <sub>5</sub> •C(C <sub>2</sub> H <sub>5</sub> ):C(C <sub>2</sub> H <sub>5</sub> )•C <sub>6</sub> H <sub>5</sub>	0.5552	Crθ(θ <sub>2</sub> ) <sub>2</sub> C <sub>5</sub> H <sub>5</sub> N
0.4647	C <sub>6</sub> H <sub>6</sub> θ <sub>4</sub>	0.5558	Co[ClC <sub>6</sub> H <sub>3</sub> (θ)CH=NC <sub>2</sub> H <sub>4</sub> N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ] <sub>2</sub>
0.4648	Vθ(C <sub>6</sub> H <sub>5</sub> CθCHCθCH <sub>3</sub> ) <sub>2</sub>	0.5571	C <sub>5</sub> H <sub>6</sub> θ <sub>4</sub> S <sub>2</sub>
0.4676	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> θ <sub>3</sub>	0.5574	C <sub>6</sub> H <sub>5</sub> •Cθ•NHCH <sub>3</sub>
0.4707	K <sub>2</sub> Pt(C <sub>2</sub> θ <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> θ	0.5580	Pb <sub>4</sub> (θH) <sub>2</sub> (Cθ <sub>3</sub> ) <sub>2</sub> Sθ <sub>4</sub>
0.4708	C <sub>13</sub> H <sub>12</sub> θ <sub>2</sub>	0.5601	Te(CH <sub>3</sub> ) <sub>2</sub> I <sub>2</sub>
0.4709	C <sub>2</sub> H <sub>5</sub> N <sub>5</sub> S	0.5609	C <sub>6</sub> H <sub>8</sub> Cl <sub>4</sub>
0.4725	(θC <sub>6</sub> H <sub>4</sub> Nθ <sub>2</sub> ) <sub>2</sub> (P•S)-θCH <sub>3</sub>	0.5618	C <sub>4</sub> Cl <sub>4</sub> N <sub>4</sub> S <sub>4</sub>
0.4727	Cu <sub>2</sub> Sθ <sub>4</sub> •5SC(NH <sub>2</sub> ) <sub>2</sub> •3H <sub>2</sub> θ	0.5632	C <sub>7</sub> H <sub>3</sub> Nθ <sub>4</sub> Ca•3H <sub>2</sub> θ
0.4732	C <sub>6</sub> H <sub>2</sub> N <sub>2</sub> θ <sub>8</sub> •6H <sub>2</sub> θ	0.5657	RbHC <sub>2</sub> θ <sub>4</sub>
0.4733	Co(C <sub>5</sub> H <sub>5</sub> N) <sub>2</sub> Br <sub>2</sub>	0.5676	H <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> S•Sθ <sub>2</sub> •CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> •2HCl•H <sub>2</sub> θ
0.4741	Zn(C <sub>5</sub> H <sub>5</sub> N) <sub>2</sub> Cl <sub>2</sub>	0.5677	2Cθ(NH <sub>2</sub> ) <sub>2</sub> •H <sub>2</sub> C <sub>2</sub> θ <sub>4</sub>
0.4753	C <sub>7</sub> H <sub>6</sub> θ <sub>2</sub> •HCl	0.5687	CdBr <sub>2</sub> [θ(C(NH <sub>2</sub> )NHCH <sub>3</sub> )] <sub>2</sub> •2.5H <sub>2</sub> θ
0.4755	C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> θ <sub>4</sub>	0.5689	C <sub>12</sub> H <sub>18</sub> θ <sub>2</sub> N <sub>4</sub> S•2HCl
0.4761	K <sub>2</sub> Pt(C <sub>2</sub> θ <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> θ	0.5695	C <sub>4</sub> H <sub>8</sub> θSe•I <sub>2</sub>
0.4776	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> Sn•Mn(Cθ) <sub>4</sub> •P(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub>	0.5713	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> θ <sub>2</sub> •2HCl
0.4812	(CH <sub>3</sub> ) <sub>2</sub> •C <sub>4</sub> H <sub>8</sub> Se <sub>2</sub>	0.5716	C <sub>12</sub> H <sub>16</sub> ClN <sub>4</sub> θS•HCl•H <sub>2</sub> θ
0.4813	C <sub>14</sub> H <sub>8</sub> Cl <sub>2</sub>	0.5717	C <sub>8</sub> H <sub>7</sub> CθθH
0.4837	Zn(C <sub>5</sub> H <sub>5</sub> N) <sub>2</sub> Cl <sub>2</sub>	0.5723	C <sub>6</sub> H <sub>4</sub> Nθ <sub>2</sub> CH <sub>3</sub>
0.4839	Zn(NCS) <sub>2</sub> •2(NH <sub>2</sub> •NH <sub>2</sub> )	0.5731	Cu[(CH <sub>3</sub> ) <sub>2</sub> C <sub>2</sub> N <sub>2</sub> θ <sub>2</sub> H] <sub>2</sub>
0.4859	(C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> θ) <sub>2</sub> •0.5C <sub>2</sub> H <sub>6</sub> θ <sub>2</sub>	0.5779	C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub> Br <sub>2</sub>
0.4865	Mn(NCS) <sub>2</sub> •2(NH <sub>2</sub> •NH <sub>2</sub> )	0.5810	CS(SH) <sub>2</sub>
0.4873	Cd(NCS) <sub>2</sub> •2(NH <sub>2</sub> •NH <sub>2</sub> )	0.5826	C <sub>12</sub> H <sub>10</sub> θ <sub>2</sub>
0.4893	Pb(θC•CH <sub>3</sub> ) <sub>4</sub>	0.5830	H <sub>2</sub> NθC-CθCH:CH•Cθ•NH•N:
0.4894	(H <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> ) <sub>3</sub> CClθ <sub>4</sub>	0.5852	Fe <sub>2</sub> (Cθ) <sub>6</sub> (C <sub>6</sub> H <sub>5</sub> •C:CH) <sub>3</sub>
0.4927	(Cl <sub>3</sub> PNCH <sub>3</sub> ) <sub>2</sub>	0.5865	N(C <sub>6</sub> H <sub>4</sub> F) <sub>3</sub>
0.4959	C <sub>8</sub> H <sub>5</sub> Nθ <sub>2</sub>		

P<sub>2</sub><sub>1</sub>/c C<sub>2</sub><sub>h</sub><sup>5</sup> No. 14 (continued)

## Organic (continued)

0.5869	C <sub>6</sub> H <sub>8</sub> Br <sub>4</sub>	0.6749	N(C <sub>6</sub> H <sub>4</sub> Cl) <sub>3</sub>
0.5874	RhH(C <sub>2</sub> H <sub>3</sub> Cl) <sub>2</sub>	0.6765	C <sub>6</sub> H <sub>7</sub> N <sub>3</sub> Cl <sub>2</sub>
0.5902	KH(C <sub>2</sub> H <sub>3</sub> Cl) <sub>2</sub>	0.6783	Ca(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub>
0.5926	C <sub>6</sub> H <sub>4</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.6790	C <sub>9</sub> H <sub>12</sub> N <sub>4</sub>
0.5932	KHC <sub>2</sub> H <sub>4</sub>	0.6806	C <sub>6</sub> H <sub>5</sub> C(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub>
0.5954	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>	0.6815	NH <sub>2</sub> (CH <sub>2</sub> ) <sub>2</sub> HS
0.5967	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub>	0.6823	C <sub>5</sub> H <sub>4</sub> N <sub>5</sub> C <sub>2</sub> H <sub>5</sub>
0.5973	(CH <sub>3</sub> ) <sub>3</sub> SHgI <sub>3</sub>	0.6824	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> S <sub>2</sub> HBr
0.6016	C <sub>4</sub> H <sub>5</sub> N <sub>2</sub>	0.6825	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> Cl <sub>2</sub>
0.6022	C <sub>7</sub> H <sub>8</sub> Cl <sub>4</sub>	0.6834	C <sub>3</sub> H <sub>7</sub> N <sub>3</sub> Cl <sub>2</sub> HBr
0.6029	C <sub>5</sub> H <sub>4</sub> NC <sub>2</sub> H <sub>5</sub>	0.6838	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> Cl <sub>2</sub>
0.6029	[(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> C <sub>4</sub> (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> Pd <sub>2</sub> Cl <sub>2</sub>	0.6844	C <sub>21</sub> H <sub>26</sub> BrN <sub>2</sub>
0.6034	[(NH <sub>2</sub> ) <sub>2</sub> CS] <sub>4</sub> TeCl <sub>2</sub> •2H <sub>2</sub> O	0.6846	C <sub>4</sub> H <sub>3</sub> N <sub>2</sub> Se <sub>2</sub>
0.6038	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> S <sub>2</sub>	0.6858	N(C <sub>6</sub> H <sub>4</sub> Br) <sub>3</sub>
0.6115	C <sub>6</sub> H <sub>4</sub> (N <sub>2</sub> ) <sub>2</sub>	0.6862	C <sub>6</sub> H <sub>2</sub> N <sub>4</sub> Na <sub>2</sub> •4H <sub>2</sub> O
0.6120	H <sub>4</sub> Fe(CN) <sub>6</sub>	0.6872	[(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> Br][BF <sub>4</sub> ]
0.6130	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> S	0.6875	Te(CH <sub>3</sub> N <sub>2</sub> S) <sub>2</sub> (C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> S) <sub>2</sub> Cl <sub>2</sub>
0.6132	C <sub>19</sub> H <sub>12</sub> Cl <sub>2</sub>	0.6883	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> :C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub>
0.6134	C <sub>10</sub> H <sub>15</sub> N <sub>2</sub>	0.6903	Te(CH <sub>3</sub> N <sub>2</sub> S) <sub>4</sub> (SCN) <sub>2</sub>
0.6135	NaCN•2H <sub>2</sub> O	0.6925	NaNH <sub>4</sub> (MoCl <sub>3</sub> •C <sub>2</sub> H <sub>4</sub> )•2H <sub>2</sub> O
0.6147	H <sub>2</sub> N•C <sub>6</sub> H <sub>4</sub> •CH(C <sub>2</sub> H <sub>5</sub> )•CH(C <sub>2</sub> H <sub>5</sub> )•C <sub>6</sub> H <sub>4</sub> •NH <sub>2</sub>	0.6928	Cu(C <sub>6</sub> H <sub>4</sub> HC <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> •4H <sub>2</sub> O
0.6164	C <sub>19</sub> H <sub>12</sub> Cl <sub>2</sub>	0.6962	Al(CH <sub>2</sub> H <sub>5</sub> ) <sub>3</sub>
0.6164	(N <sub>2</sub> ) <sub>4</sub> Fe <sub>2</sub> S <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	0.6974	CdCl <sub>2</sub> •C(CH <sub>3</sub> ) <sub>2</sub> NHCH <sub>3</sub>
0.6177	C <sub>30</sub> H <sub>18</sub> Cl <sub>2</sub>	0.6988	C <sub>30</sub> H <sub>20</sub>
0.6180	C <sub>6</sub> H <sub>5</sub> N <sub>2</sub>	0.7006	C <sub>32</sub> H <sub>36</sub> CuN <sub>4</sub>
0.6182	Zn(C <sub>6</sub> H <sub>4</sub> N•C <sub>5</sub> H <sub>3</sub> N•C <sub>5</sub> H <sub>3</sub> N•C <sub>5</sub> H <sub>4</sub> N)Cl <sub>2</sub> •2H <sub>2</sub> O	0.7023	TiCl <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
0.6206	C <sub>10</sub> H <sub>4</sub> Br <sub>2</sub> Cl <sub>2</sub>	0.7028	CH <sub>6</sub> N <sub>4</sub> •HCl
0.6209	ZnCl <sub>2</sub> •C <sub>12</sub> H <sub>8</sub> N <sub>2</sub>	0.7035	C <sub>4</sub> H <sub>6</sub> Li•C <sub>4</sub> H <sub>6</sub> Li
0.6215	(CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.7078	Cd(N <sub>2</sub> ) <sub>2</sub> •4[(NH <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ]
0.6225	CH <sub>3</sub> •C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> Cl <sub>2</sub>	0.7086	C <sub>20</sub> H <sub>20</sub>
0.6235	Fe <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>6</sub> •C <sub>14</sub> H <sub>13</sub> N	0.7087	Cu(NH <sub>3</sub> ) <sub>2</sub> Cl <sub>3</sub>
0.6245	H <sub>2</sub> C <sub>6</sub> H <sub>4</sub> •CH(C <sub>2</sub> H <sub>5</sub> )•CH(C <sub>2</sub> H <sub>5</sub> )•C <sub>6</sub> H <sub>4</sub> •H	0.7100	(CH <sub>3</sub> ) <sub>2</sub> GaH
0.6250	V(CH <sub>3</sub> ) <sub>3</sub>	0.7105	Co(CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •4H <sub>2</sub> O
0.6273	C <sub>30</sub> H <sub>28</sub> CuN <sub>2</sub> Cl <sub>2</sub>	0.7116	C <sub>22</sub> H <sub>26</sub> Cl <sub>16</sub>
0.6275	C <sub>6</sub> H <sub>7</sub> N <sub>5</sub>	0.7128	Cu[SCSN(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> ] <sub>2</sub>
0.6287	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> Cl <sub>2</sub>	0.7168	Cu(CH <sub>3</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •2H <sub>2</sub> O
0.6291	Te(C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> S) <sub>2</sub> I <sub>2</sub>	0.7171	Ni(CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •4H <sub>2</sub> O
0.6316	Cu(C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>2</sub> (N <sub>2</sub> ) <sub>2</sub>	0.7179	SbCl <sub>5</sub> •HC <sub>6</sub> H <sub>5</sub> (CH <sub>3</sub> ) <sub>2</sub>
0.6321	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> S <sub>2</sub>	0.7182	C <sub>8</sub> H <sub>12</sub> N <sub>4</sub> S
0.6327	Zn[SC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> (CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.7195	C <sub>4</sub> H <sub>8</sub> Se <sub>2</sub> •C <sub>2</sub> I <sub>4</sub>
0.6338	C <sub>6</sub> H <sub>10</sub> N•S <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> I	0.7226	Mg(CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •4H <sub>2</sub> O
0.6341	C <sub>15</sub> H <sub>25</sub> Br <sub>2</sub>	0.7274	Cu(NH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
0.6341	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>6</sub> C <sub>6</sub> H <sub>3</sub> CH <sub>3</sub>	0.7274	Se <sub>2</sub> (CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> S <sub>2</sub> ) <sub>2</sub>
0.6348	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> Se <sub>2</sub>	0.7288	C <sub>6</sub> H <sub>5</sub> •C <sub>7</sub> H <sub>7</sub> •Cr(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub>
0.6352	C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub> S	0.7300	Ca(N <sub>2</sub> ) <sub>2</sub> •4[(NH <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ]
0.6369	(CH <sub>3</sub> Se <sub>2</sub> S) <sub>2</sub>	0.7312	C <sub>6</sub> H <sub>4</sub> Cl <sub>8</sub>
0.6379	C <sub>10</sub> H <sub>8</sub> N <sub>4</sub> Cl <sub>2</sub>	0.7320	C <sub>12</sub> H <sub>8</sub> Cl <sub>6</sub>
0.6403	C <sub>6</sub> H <sub>7</sub> N <sub>3</sub> Cl <sub>2</sub> •2HCl	0.7348	SnCl <sub>3</sub> •CH <sub>3</sub> •CH <sub>3</sub> OH
0.6404	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> •CdBr <sub>2</sub>	0.7351	Mn <sub>3</sub> [(CH <sub>3</sub> •CH <sub>2</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ] <sub>2</sub> •10H <sub>2</sub> O
0.6404	CaC <sub>2</sub> Cl <sub>4</sub> •H <sub>2</sub> O	0.7360	(CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
0.6413	Fe <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub>	0.7365	BrC <sub>6</sub> H <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> NHS <sub>2</sub> C <sub>6</sub> H <sub>5</sub>
0.6429	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> Cl	0.7366	Cu(C <sub>5</sub> H <sub>5</sub> N <sub>2</sub> )Cl <sub>2</sub>
0.6429	Cu(CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •3H <sub>2</sub> O	0.7371	C <sub>13</sub> H <sub>10</sub> N <sub>4</sub> Cl <sub>6</sub>
0.6430	(C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> ) <sub>2</sub> Cu	0.7379	Mn[Mn(CH <sub>2</sub> ) <sub>2</sub> H(CH <sub>2</sub> N(CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> •8H <sub>2</sub> O
0.6461	(C <sub>6</sub> H <sub>7</sub> N <sub>2</sub> ) <sub>2</sub>	0.7382	C <sub>5</sub> H <sub>5</sub> Mo(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> F <sub>7</sub>
0.6528	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> S•HCl	0.7385	C <sub>6</sub> H <sub>5</sub> Br <sub>3</sub> •H <sub>2</sub> O
0.6548	C <sub>16</sub> H <sub>12</sub>	0.7387	(NH <sub>2</sub> C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(C <sub>2</sub> H <sub>4</sub> NH <sub>2</sub> ) <sub>2</sub> [Co(CH <sub>3</sub> ) <sub>2</sub> I <sub>2</sub> ]
0.6549	Cu(C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> ) <sub>2</sub> •C <sub>6</sub> (N <sub>2</sub> ) <sub>3</sub>	0.7403	C <sub>6</sub> H <sub>8</sub> Cl <sub>4</sub> S <sub>2</sub>
0.6550	[(CH <sub>3</sub> ) <sub>2</sub> AsC <sub>6</sub> H <sub>4</sub> ] <sub>2</sub> AsCH <sub>3</sub> CuMn(C <sub>6</sub> H <sub>5</sub> ) <sub>5</sub>	0.7409	CuS <sub>4</sub> •(CH <sub>2</sub> ) <sub>6</sub> N <sub>4</sub> •H <sub>2</sub> S <sub>4</sub>
0.6550	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub>	0.7423	K <sub>2</sub> (Pd(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> ) <sub>2</sub> •4H <sub>2</sub> O
0.6552	(CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •H <sub>2</sub> O	0.7443	C <sub>15</sub> H <sub>13</sub> Br
0.6554	LaH[(CH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ] <sub>2</sub> •7H <sub>2</sub> O	0.7449	I•C <sub>6</sub> H <sub>4</sub> •C <sub>6</sub> H <sub>5</sub>
0.6565	C <sub>26</sub> H <sub>20</sub> I <sub>2</sub>	0.7450	NH <sub>4</sub> HC <sub>5</sub> H <sub>5</sub>
0.6573	Fe(C <sub>6</sub> H <sub>5</sub> N <sub>2</sub> ) <sub>3</sub>	0.7459	S <sub>2</sub> (CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> S <sub>2</sub> ) <sub>2</sub>
0.6576	C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> Cl	0.7478	RbHC <sub>5</sub> H <sub>5</sub>
0.6586	[(CH <sub>3</sub> ) <sub>3</sub> Pt•CH <sub>3</sub> •C <sub>6</sub> H <sub>5</sub> •CH <sub>3</sub> •C <sub>6</sub> H <sub>5</sub> ] <sub>2</sub>	0.7484	HC <sub>6</sub> H <sub>5</sub>
0.6603	C <sub>5</sub> H <sub>8</sub> Cl <sub>2</sub>	0.7500	C <sub>14</sub> H <sub>10</sub> N <sub>2</sub> Cl <sub>2</sub>
0.6613	C <sub>20</sub> H <sub>12</sub>	0.7527	Fe(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> C <sub>4</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub>
0.6639	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> S	0.7587	Ca(CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> )Cl•5H <sub>2</sub> O
0.6653	CuC <sub>3</sub> H <sub>5</sub> N <sub>2</sub> •3H <sub>2</sub> O	0.7591	C <sub>10</sub> H <sub>8</sub> N <sub>4</sub> Cl <sub>2</sub>
0.6670	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> Cl <sub>2</sub>	0.7593	C <sub>8</sub> H <sub>8</sub> Cl <sub>3</sub> S <sub>2</sub>
0.6684	Te(CH <sub>3</sub> N <sub>2</sub> S) <sub>2</sub> (C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> S) <sub>2</sub> Br <sub>2</sub>	0.7598	(C <sub>16</sub> H <sub>12</sub> ) <sub>2</sub>
0.6742	C <sub>15</sub> H <sub>16</sub> Cl <sub>2</sub>	0.7619	NH <sub>2</sub> (CH <sub>2</sub> ) <sub>6</sub> NH <sub>2</sub> •2HI

$P2_1/c$   $C_{2h}^5$  No. 14 (continued)

Organic (continued)			
0.7637	$C_{16}H_{22}Cl_4 \cdot C_8H_{13}NO$	0.8607	$BrCH_3C_6H_3NO_2$
0.7652	$Ni(SC_2H_5)_2$	0.8630	$(CH_4N_2O)_2 \cdot C_7H_{12}O_4$
0.7653	$C_6Cl_6O$	0.8639	$(NH_2)_2C_6Cl_2O_2$
0.7681	$C_{12}H_4Cl_4N_2$	0.8639	$C_2H_4Cl_2N_6$
0.7700	$Fe[C_5H_4 \cdot CH_2(\theta H)CH_3]_2$	0.8652	$C_{13}H_9N$
0.7702	$SnBr_3\theta CH_3 \cdot CH_3\theta H$	0.8657	$C_8H_{10}\theta$
0.7714	$NaHC\theta_3$	0.8670	$C_{20}H_{21}NO_4 \cdot HBr$
0.7720	$[Cu(NH_2CH_2CH_2NH_2)_2]Cl_2 \cdot H_2\theta$	0.8672	$Pb[SC(NH_2)_2](C_2H_3O_2)_2$
0.7726	$H_2N-C\theta-N-N-C\theta-NH_2$	0.8672	$Cl_2C_6H_3 \cdot NClC\theta NCl \cdot C_6H_3Cl_2$
0.7736	$C_{10}H_{18}(NH_2)_2 \cdot 2HCl$	0.8680	$C_{28}H_{32}O_4Si_4$
0.7742	$NaHC\theta_3$	0.8687	$C_{36}H_{38}N_2O_2$
0.7751	$Cu(C_4H_6N_2)_4(N\theta_3)_2$	0.8697	$(CH_2-CH_2 \cdot C\theta\theta H)_2(NH_2-CH_2)_2$
0.7756	$C_{14}H_6N\theta_2$	0.8713	$C_8H_8N\theta_3Cl$
0.7757	$(C_2H_2\theta_8^{16})_2$	0.8728	$N(CH_3)_4I_9$
0.7770	$P(C_6H_5)_3$	0.8766	$Ni(NH_2CH_2CH_2NH_2)_2ClBr$
0.7802	$C_6H_8(\theta H)_6$	0.8767	$(C_3H_6N_2S)_2CuCl$
0.7806	$C_2H_3N_3S_2HBr$	0.8791	$C_{24}H_{16}$
0.7808	$C_{20}H_{19}N\theta_5$	0.8816	$C_4H_4Cl_4\theta_2$
0.7831	$[Cu(NH_2CH_2CH_2NH_2)_2]Br_2 \cdot H_2\theta$	0.8819	$C_6H_2Br_4$
0.7837	$[Co(C_2H_4(NH_2)_2)_2(N\theta_2)_2]N\theta_3$	0.8851	$Cu(CH_3CH_2C\theta\theta)_2 \cdot H_2\theta$
0.7838	$[Fe(C\theta)_4]_3$	0.8862	$C_8H_{10}N_4O_2 \cdot H_2\theta$
0.7859	$C_{19}H_{22}\theta_2$	0.8877	$C_6H_8Br_2\theta_4$
0.7875	$Hg(SCN)_4 \cdot Cu(NH_2 \cdot CH_2CH_2 \cdot NH_2)_2$	0.8887	$C_{20}H_{10}\theta_4$
0.7880	$Cu_2(\theta H)_2C\theta_3$	0.8902	$(C_4H_5N\theta)_2$
0.7887	$C_5HBr_3C_6H_4\theta CH_3$	0.8904	$C_{18}H_{22}N_2S \cdot HCl$
0.7921	$Cu(C_{10}H_{10}N\theta)_2$	0.8906	$Cu(C_2H_3\theta_3)_2$
0.7921	$Ni(CH_3N_2S_2)(HN_2S_2)$	0.8907	$RuCl_2[P(C_6H_5)_3]_3$
0.7925	$C_4H_5N_3\theta \cdot H_2\theta$	0.8998	$C_6H_2Cl_4$
0.7930	$C_4H_4N_2\theta_2S$	0.9006	$HgCl_2 \cdot C_3N_3\theta_3(C_2H_3)_3$
0.7939	$C_8H_6Cl_2$	0.9011	$(C_6H_5)_4AsRuCl_4(H_2\theta)_2 \cdot H_2\theta$
0.7974	$C_5HCl_3C_6H_4\theta CH_3$	0.9026	$C_6H_2Cl_4$
0.8014	$C_{23}H_{35}Br\theta_9$	0.9034	$C_{14}H_{12} \cdot Cr(C\theta)_3$
0.8020	$Ni[NH_2 \cdot (CH_3)_2C \cdot C\theta\theta]_2 \cdot 4H_2\theta$	0.9039	$CH_3\theta \cdot Cl \cdot C_6H_3 \cdot CH : CH \cdot C\theta\theta H$
0.8025	$(CH_3C\theta\theta CH_2CH_2N(CH_3)_3)Br$	0.9048	$(C\theta\theta H)_2$
0.8037	$Hg(CN)_2 \cdot SC(NH_2)_2$	0.9057	$C_6H_2Cl_4$
0.8042	$H\theta\theta C \cdot CH_2\theta \cdot C_6H_4 \cdot C\theta \cdot NH \cdot CH_2 \cdot CH : CH_2$	0.9062	$C_{15}H_{11}N_3$
0.8045	$C_{14}H_8\theta_2$	0.9070	$C_5H_5\theta_5 \cdot C_5H_4C\theta C_6H_5$
0.8050	$Cl_3C_6H_2CN$	0.9082	$C_{17}H_{25}NOHCl$
0.8053	$LiH_2C\theta_2CH_2C\theta RC\theta_2CH_2C\theta_2$	0.9096	$H_{10}Br_4H_6C_2(CH_3)_2$
0.8057	$CH_3\theta \cdot C_6H_4 \cdot CH : CBr \cdot C\theta\theta H$	0.9120	$Ni(NH_2CS_2)_2$
0.8062	$(C_{16}H_{12})_2$	0.9126	$C_{24}H_{19}N\theta_2Pb$
0.8077	$K_3Fe(CN)_6$	0.9149	$C_4H_5N_3\theta$
0.8077	$K_3Co(CN)_6$	0.9158	$C_8H_{10}Br_2\theta_4$
0.8096	$C_{13}H_{11}\theta_2P$	0.9163	$C_5H_{10}N_2\theta S$
0.8099	$Rh_3Fe(CN)_6$	0.9165	$Pt(CH_3)_3I$
0.8156	$C_{12}H_8\theta_2S_2$	0.9171	$(C_5H_5)Fe(C_5H_4C\theta \cdot C_6H_5)$
0.8164	$Cu[NH_2C\theta NHNH_2]_2Cl_2$	0.9207	$Cl_2 \cdot C_6H_3 \cdot CH : CH \cdot C\theta\theta H$
0.8170	$(C_{12}H_{16}N\theta)_2Pd$	0.9211	$As_5(CH_3)_5$
0.8181	$C_{10}H_{11}N\theta_4S_2$	0.9224	$ClSbS_2(CH_2)_2$
0.8203	$NH_2 \cdot CH_2 \cdot C\theta \cdot NH \cdot CH_2 \cdot C\theta\theta H$	0.9226	$C_{10}H_{10}N_2\theta$
0.8242	$C_5H_5Co(CH_3C_2CH_3)_2C\theta$	0.9245	$CH_2\theta H \cdot C(CH_3)_2 \cdot CH_2\theta H$
0.8259	$Cu(NH_2 \cdot CH_2 \cdot CH_2 \cdot NH_2)_2(N\theta_3)_2$	0.9259	$C_6H_4BrN\theta_2$
0.8276	$NaH_2C\theta_2CH_2C\theta HC\theta_2CH_2C\theta_2$	0.9274	$C_{12}H_4N_7\theta_{12}Rb$
0.8278	$C_{18}H_{16}\theta_4$	0.9277	$CNCH_2C\theta NHNH_2$
0.8291	$C_{20}H_{21}N\theta_4HCl$	0.9282	$C_3H_{11}Br_{10}Cl_3$
0.8300	$C_{10}H_{18}CoN_7\theta_4S_2 \cdot 3H_2\theta$	0.9315	$C_6H_{12}N_4 \cdot 2Br$
0.8337	$C_{10}H_{30}Al_2\theta_2Si_2$	0.9315	$C_{12}H_4N_7\theta_{12}K$
0.8358	$C_4H_4N_2\theta_2$	0.9316	$C_6H_{10}N_2\theta_3$
0.8369	$C_{14}H_6Br_2\theta_2$	0.9322	$(CH_3)_2CHCH_2CH(NH_2)C\theta NFCH_2C\theta NHCH_2C\theta\theta H$
0.8394	$Cu(C_7H_5\theta_2)_2$	0.9336	$(C\theta)_3Fe(C_6H_8)Fe(C\theta)_3$
0.8414	$C_3H_7\theta C_6H_4N\theta_2$	0.9346	$(C_6H_5)_2PS(\theta CH_3)$
0.8422	$C_4H_4N_6\theta \cdot HCl \cdot H_2\theta$	0.9354	$C_8H_{12}N_6S_4Te$
0.8428	$CuCN \cdot NH_3$	0.9377	$[(N\theta_2)_3C_6H_2]_2NK$
0.8430	$ClC_6H_3(C\theta)_2C_6H_3Cl$	0.9391	$Fe[SC(NHCH_2)_2]_2Cl_2$
0.8431	$CH_2(NH_2)C\theta NHCH_2C\theta\theta H$	0.9398	$C_6H_4ClN\theta_2$
0.8448	$C_3H_3e_3Na$	0.9455	$K(C_4H_2N_3\theta_4) \cdot 2H_2\theta$
0.8452	$P\theta HCl[P(C_6H_5)_2C_2H_5]_2$	0.9455	$C_8H_5N_2\theta_2Cl$
0.8462	$B_4H_6C_2H_2$	0.9457	$N : N \cdot C_6H_4 \cdot S\theta_3$
0.8510	$CH_3C\theta NHCH_2C\theta\theta H$	0.9512	$Te(C_3H_6N_2S)_2(S_2\theta_2CH_3)_2$
0.8516	$C_{10}H_{30}N_2S_{14}$	0.9516	$C_6H_6Cl_6$
0.8530	$C_6H_5CH \cdot NNHC_6H_5$	0.9549	$Pt[P(C_2H_5)_3]_2Cl_2$
0.8531	$C_8H_8N\theta_3Br$	0.9569	$C_6H_2Br_4$
0.8558	$NH_2 \cdot C_6H_4 \cdot As\theta(\theta H)_2$	0.9590	$Cd[SC(NHCH_2)_2]_2Cl_2$
0.8561	$C_4N_2 \cdot NH_2Cl_2H$	0.9590	$Ni(NH_2CH_2CH_2NH_2)_2(CNS)Br$

P<sub>2</sub>/c C<sub>2h</sub><sup>5</sup> No. 14 (continued)

## Organic (continued)

0.9594	Ni <sub>3</sub> (NO <sub>2</sub> ) <sub>2</sub> (C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> ) <sub>6</sub> (ClO <sub>4</sub> ) <sub>4</sub>	1.0439	C <sub>26</sub> H <sub>26</sub> Cl <sub>6</sub>
0.9603	C <sub>16</sub> H <sub>21</sub> NO <sub>3</sub>	1.0441	C <sub>7</sub> H <sub>6</sub> BrNO <sub>2</sub>
0.9626	Ni[(CH <sub>3</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ] <sub>2</sub> (NO <sub>2</sub> ) <sub>2</sub>	1.0447	K <sub>2</sub> (Cu(NHC <sub>6</sub> NHCO <sub>2</sub> NH) <sub>2</sub> ) <sub>4</sub> ·4H <sub>2</sub> O
0.9635	C <sub>30</sub> H <sub>8</sub> NNaO <sub>3</sub> S <sub>4</sub> ·4H <sub>2</sub> O	1.0490	Co(C <sub>2</sub> N <sub>2</sub> O <sub>2</sub> H <sub>4</sub> ) <sub>3</sub> ·2H <sub>2</sub> O
0.9658	ZnCl <sub>2</sub> ·2C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>	1.0502	(C <sub>8</sub> H <sub>6</sub> )Fe(CO) <sub>3</sub> BF <sub>4</sub>
0.9661	[(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> P] <sub>2</sub> NiBr <sub>2</sub>	1.0512	C <sub>6</sub> H <sub>5</sub> SC <sub>6</sub> H <sub>4</sub> NO <sub>2</sub>
0.9661	Co[(CH <sub>3</sub> ) <sub>3</sub> P <sub>2</sub> ] <sub>2</sub> (NO <sub>2</sub> ) <sub>2</sub>	1.0530	NH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> OS <sub>2</sub>
0.9662	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> P <sub>3</sub> N <sub>3</sub> Cl <sub>4</sub>	1.0536	[C <sub>11</sub> H <sub>10</sub> O <sub>2</sub> S]
0.9674	Co(NO <sub>2</sub> ) <sub>3</sub> ·C <sub>2</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>	1.0554	(C <sub>5</sub> H <sub>5</sub> )P(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> FeC(C <sub>6</sub> H <sub>5</sub> )
0.9674	(CH <sub>3</sub> CH <sub>2</sub> ) <sub>3</sub> P-CSS	1.0565	(CH <sub>3</sub> ) <sub>2</sub> S <sub>2</sub> ·BF <sub>3</sub>
0.9680	CuK(CN) <sub>2</sub>	1.0568	CH <sub>3</sub> ·C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> ·HCl
0.9681	Te(C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> S) <sub>3</sub> (ClO <sub>4</sub> ) <sub>2</sub>	1.0579	Cl(NO <sub>2</sub> )C <sub>6</sub> H <sub>3</sub> ·CH <sub>3</sub>
0.9685	Te[(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> PS <sub>2</sub> ] <sub>2</sub>	1.0592	[(NH <sub>2</sub> ) <sub>2</sub> (CH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> Cl <sub>2</sub> CoCl
0.9693	Se[(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> PS <sub>2</sub> ] <sub>2</sub>	1.0595	CoCl <sub>2</sub> ·NC <sub>5</sub> H <sub>4</sub> CH <sub>2</sub> NNHC <sub>5</sub> H <sub>4</sub> N
0.9718	C <sub>9</sub> H <sub>12</sub> N <sub>4</sub> O	1.0611	CH <sub>3</sub> SgCl
0.9741	Pt[P(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> ] <sub>2</sub> Br <sub>2</sub>	1.0639	C <sub>7</sub> H <sub>6</sub> ClNO <sub>2</sub>
0.9763	C <sub>6</sub> H <sub>4</sub> [C(CH <sub>3</sub> ) <sub>3</sub> ] <sub>2</sub>	1.0646	(C <sub>8</sub> H <sub>12</sub> NiCl <sub>2</sub> ) <sub>2</sub> ·C <sub>6</sub> H <sub>6</sub>
0.9779	(C <sub>6</sub> H <sub>5</sub> SPS <sub>2</sub> ) <sub>2</sub>	1.0649	[Co(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> Cl <sub>2</sub> ] <sub>2</sub> NO <sub>3</sub>
0.9783	Se[(CH <sub>3</sub> ) <sub>2</sub> PS <sub>2</sub> ] <sub>2</sub>	1.0653	C <sub>28</sub> H <sub>22</sub> N <sub>2</sub>
0.9794	Ni(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> (NCS)Cl	1.0656	(C <sub>11</sub> H <sub>9</sub> O <sub>2</sub> ) <sub>2</sub> Ni
0.9795	[(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> Sn] <sub>6</sub> ·2[(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>4</sub> ]	1.0679	C <sub>7</sub> H <sub>6</sub> ·6Fe(CO) <sub>3</sub>
0.9816	C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	1.0687	C <sub>8</sub> H <sub>12</sub> S <sub>6</sub>
0.9842	C <sub>4</sub> H <sub>5</sub> ClN <sub>4</sub>	1.0699	DCH(OH)C <sub>6</sub> H <sub>5</sub> Cl
0.9861	C <sub>18</sub> H <sub>10</sub> Cr <sub>2</sub> O <sub>6</sub>	1.0711	CH <sub>2</sub> :CHCH <sub>2</sub> NH·CS·NH <sub>2</sub>
0.9865	C <sub>22</sub> H <sub>12</sub>	1.0712	C <sub>23</sub> H <sub>16</sub> O <sub>3</sub>
0.9884	B <sub>10</sub> Cl <sub>10</sub> C <sub>2</sub> H <sub>2</sub>	1.0724	(C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub> ) <sub>3</sub> ·C <sub>12</sub> H <sub>8</sub> (OH) <sub>2</sub>
0.9899	Os <sub>3</sub> (CO) <sub>12</sub>	1.0737	C <sub>19</sub> H <sub>18</sub> O <sub>6</sub>
0.9906	ClC <sub>7</sub> H <sub>6</sub> N(NO)N:C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> ·H <sub>2</sub> O	1.0742	H <sub>2</sub> CC·CH:CH·CH·C <sub>6</sub> H <sub>5</sub>
0.9913	Fe <sub>3</sub> (CO) <sub>8</sub> (C <sub>6</sub> H <sub>5</sub> C <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	1.0745	(CH <sub>3</sub> ) <sub>3</sub> S <sub>2</sub> AlBr <sub>2</sub>
0.9939	PdCl <sub>2</sub> (CH <sub>3</sub> S <sub>2</sub> CH <sub>3</sub> ) <sub>2</sub>	1.0759	H <sub>2</sub> C·C <sub>6</sub> H <sub>4</sub> ·C(C <sub>2</sub> H <sub>5</sub> ):C(C <sub>2</sub> H <sub>5</sub> )C <sub>6</sub> H <sub>4</sub> OH·C <sub>6</sub> H <sub>5</sub>
0.9940	[(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NCS] <sub>2</sub> Ni	1.0771	C <sub>3</sub> H <sub>5</sub> Fe(CO) <sub>3</sub> I
0.9943	C <sub>2</sub> H <sub>2</sub> B <sub>10</sub> Cl <sub>10</sub>	1.0788	CH <sub>3</sub> S <sub>2</sub> SK
0.9994	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub> ·HBr	1.0835	(C <sub>5</sub> H <sub>5</sub> )Fe(C <sub>5</sub> H <sub>4</sub> ·CO·C <sub>6</sub> H <sub>3</sub> (OH)(OCH <sub>3</sub> ))
1.0000	C <sub>11</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> S	1.0844	(C <sub>21</sub> H <sub>15</sub> N <sub>3</sub> )Ni(NO <sub>2</sub> ) <sub>2</sub> ·2H <sub>2</sub> O
1.0010	Ni[(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> PS <sub>2</sub> ] <sub>2</sub>	1.0860	SnCl <sub>4</sub> ·2(C <sub>4</sub> H <sub>8</sub> S)
1.0037	Cu(HCO <sub>2</sub> ) <sub>2</sub> ·4H <sub>2</sub> O	1.0871	[C <sub>3</sub> H <sub>5</sub> Fe(CO) <sub>3</sub> ] <sub>2</sub> I
1.0040	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub>	1.0876	Ni(NO <sub>2</sub> ) <sub>3</sub> ·C <sub>2</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub>
1.0045	C <sub>12</sub> H <sub>4</sub> K <sub>2</sub> N <sub>4</sub>	1.0896	[(C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> As] <sub>2</sub> (HgCl <sub>2</sub> ) <sub>3</sub>
1.0052	C <sub>12</sub> H <sub>8</sub> N <sub>2</sub>	1.0907	I(NO <sub>2</sub> )C <sub>6</sub> H <sub>3</sub> ·CH <sub>3</sub>
1.0057	[(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NCS] <sub>2</sub> Ni	1.0935	C <sub>7</sub> H <sub>9</sub> N <sub>5</sub> O·C <sub>4</sub> H <sub>4</sub> BrN <sub>3</sub> O
1.0071	[TiCl <sub>2</sub> (C <sub>5</sub> H <sub>5</sub> )] <sub>2</sub> O	1.0948	Na <sub>2</sub> C <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O <sub>2</sub>
1.0096	C <sub>16</sub> H <sub>10</sub>	1.0950	[BrMn(CO) <sub>4</sub> ] <sub>2</sub>
1.0111	(CO) <sub>4</sub> (CH <sub>2</sub> :CH·CN)Fe	1.0956	C <sub>6</sub> H <sub>5</sub> ·6K <sub>3</sub> ·H <sub>2</sub> O
1.0113	C <sub>18</sub> H <sub>19</sub> IN <sub>2</sub>	1.0959	C <sub>30</sub> H <sub>20</sub> N <sub>4</sub> Na <sub>2</sub> O <sub>4</sub>
1.0130	C <sub>16</sub> H <sub>32</sub> N <sub>4</sub> ·Ni(ClO <sub>4</sub> ) <sub>2</sub>	1.0963	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O·HCl·2H <sub>2</sub> O
1.0132	C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> S·HCl	1.0964	C <sub>5</sub> H <sub>5</sub> N·HN <sub>2</sub> O
1.0133	Ni[(CH <sub>3</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub> (NO <sub>2</sub> ) <sub>2</sub>	1.0965	C <sub>6</sub> H <sub>6</sub> NC <sub>2</sub> Cl <sub>3</sub>
1.0144	[NiN(CH <sub>2</sub> ·CH <sub>2</sub> ·CH <sub>2</sub> ·NH <sub>2</sub> ) <sub>3</sub> ](SCN) <sub>2</sub>	1.1032	Co(CH <sub>3</sub> S(CH <sub>2</sub> ) <sub>2</sub> SC <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> (ClO <sub>4</sub> ) <sub>2</sub>
1.0147	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	1.1047	(C <sub>5</sub> H <sub>4</sub> ·C <sub>5</sub> H <sub>4</sub> )Fe <sub>2</sub> (CH <sub>3</sub> CO·C <sub>5</sub> H <sub>4</sub> ) <sub>2</sub>
1.0160	Cu(C <sub>2</sub> H <sub>5</sub> ·CH <sub>3</sub> ·C <sub>2</sub> N <sub>2</sub> O <sub>2</sub> H <sub>2</sub> ) <sub>2</sub>	1.1048	UCl(C <sub>5</sub> H <sub>5</sub> ) <sub>3</sub>
1.0177	CH <sub>3</sub> CH(NH <sub>2</sub> )CO <sub>2</sub> H·HCl	1.1050	C <sub>6</sub> H <sub>18</sub> N <sub>2</sub> Cl <sub>2</sub>
1.0178	(C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O) <sub>2</sub>	1.1056	CH <sub>3</sub> C(NH <sub>2</sub> )S
1.0179	IrCl(CO)(SO <sub>2</sub> )(P(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> ) <sub>2</sub>	1.1064	Te(C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> S) <sub>2</sub> I <sub>2</sub>
1.0180	Zn <sub>4</sub> [S <sub>2</sub> P(O <sub>2</sub> CH <sub>3</sub> ) <sub>2</sub> ] <sub>6</sub> O	1.1079	Pt <sub>2</sub> (SCN) <sub>2</sub> Cl <sub>2</sub> [(C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> P] <sub>2</sub>
1.0187	Ni(CH <sub>3</sub> ·C <sub>2</sub> H <sub>5</sub> ·C <sub>2</sub> N <sub>2</sub> O <sub>2</sub> H <sub>2</sub> ) <sub>2</sub>	1.1093	(C <sub>6</sub> H <sub>4</sub> Br) <sub>2</sub>
1.0195	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> ·HBr	1.1094	(NO <sub>2</sub> ) <sub>4</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>
1.0198	C <sub>20</sub> H <sub>14</sub> N <sub>4</sub>	1.1098	C <sub>5</sub> H <sub>11</sub> O <sub>2</sub> NS·HCl·H <sub>2</sub> O
1.0204	C <sub>12</sub> H <sub>4</sub> N <sub>7</sub> O <sub>12</sub> K	1.1100	C <sub>6</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> Pd
1.0217	(C <sub>6</sub> H <sub>5</sub> CO) <sub>2</sub> S <sub>2</sub>	1.1102	C <sub>5</sub> H <sub>16</sub> ClN <sub>5</sub> NiO <sub>4</sub> S
1.0222	C <sub>6</sub> H <sub>3</sub> (NO <sub>2</sub> ) <sub>2</sub> O·C <sub>10</sub> H <sub>6</sub> NH <sub>2</sub> Br	1.1123	C <sub>2</sub> H <sub>2</sub> N <sub>4</sub>
1.0238	C <sub>8</sub> H <sub>15</sub> NO <sub>2</sub> ·HBr	1.1127	C <sub>14</sub> H <sub>10</sub>
1.0250	C <sub>15</sub> H <sub>14</sub> O <sub>3</sub>	1.1136	[(C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> As] <sub>2</sub> (CdI <sub>2</sub> ) <sub>2</sub>
1.0277	H <sub>2</sub> C·C <sub>6</sub> H <sub>4</sub> ·C <sub>6</sub> H <sub>5</sub>	1.1152	C <sub>5</sub> H <sub>5</sub> NO <sub>2</sub> I <sub>2</sub>
1.0280	Ca(P <sub>2</sub> O <sub>7</sub> ) <sub>2</sub> ·2CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	1.1156	C <sub>6</sub> H <sub>18</sub> N <sub>2</sub> Br <sub>2</sub>
1.0288	Mn(P <sub>2</sub> O <sub>7</sub> ) <sub>2</sub> (CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	1.1158	C <sub>25</sub> H <sub>27</sub> N
1.0335	C <sub>16</sub> H <sub>11</sub> CrN <sub>3</sub> O <sub>10</sub>	1.1176	CH <sub>3</sub> ·C <sub>6</sub> H <sub>4</sub> ·CH:CH·C <sub>6</sub> H <sub>5</sub>
1.0346	C <sub>16</sub> H <sub>23</sub> NO <sub>2</sub> ·HCl	1.1182	C <sub>6</sub> Cl <sub>4</sub> [ <sub>2</sub> Sn(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> ] <sub>2</sub>
1.0354	[(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> C <sub>4</sub> O <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ] <sub>2</sub> Pd <sub>2</sub> Cl <sub>2</sub>	1.1188	C <sub>8</sub> H <sub>17</sub> NO
1.0370	(C <sub>10</sub> H <sub>6</sub> ) <sub>2</sub>	1.1191	C <sub>10</sub> H <sub>11</sub> NO <sub>4</sub>
1.0383	C <sub>6</sub> H <sub>4</sub> O <sub>2</sub>	1.1233	C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> NiO <sub>2</sub>
1.0384	C <sub>6</sub> H <sub>8</sub> O <sub>4</sub>	1.1258	[Co(NO <sub>2</sub> )[S <sub>2</sub> C·N(CH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub> ]
1.0423	Cu(NCS) <sub>2</sub> ·2(C <sub>5</sub> H <sub>5</sub> N)	1.1265	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> Sn(I)(CH <sub>2</sub> ) <sub>4</sub> (I)Sn(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
1.0427	C <sub>21</sub> H <sub>23</sub> BrO <sub>4</sub>	1.1302	C <sub>6</sub> H <sub>5</sub> ·C <sub>4</sub> HCl <sub>2</sub> O
1.0433	C <sub>10</sub> H <sub>13</sub> ClIN <sub>5</sub>	1.1315	2C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub> ·ZnBr <sub>2</sub>

$P2_1/c$   $C_{2h}^5$  No. 14 (continued)

## Organic (continued)

1.1349	$Rb_3C_8O_2CH_2C_6H_5C_2H_2C_6O_2 \cdot H_2O$	1.2261	$C_{22}H_{14}$
1.1365	$C_6H_5NO_2$	1.2264	$Ag_2CN_2$
1.1370	$(C_6H_4Cl)_2NH$	1.2278	$(C_{13}H_{12}NO)_2Cu$
1.1384	$C_{20}H_{28}O_{13} \cdot H_2O$	1.2279	$C_{10}H_8O_2S$
1.1392	$Zn(N_2H_4)_2(NH_2 \cdot NHC_6H_5)_2$	1.2301	$Ni(C_2H_8N_2)_2Cl_2$
1.1393	$[(C_2H_5)_3P]_2(CdBr_2)_2$	1.2319	$(C_6H_5CO)_3CN \cdot NC_6H_4Br$
1.1402	$C_{20}H_{20}ClN$	1.2332	$C_{21}H_{15}Cl_4$
1.1410	$C_6H_8N_2O_2S$	1.2367	$NO_2 \cdot C_6H_4 \cdot COOH$
1.1411	$Rb(C_6H_5)_3$	1.2373	$(CO)_3FeOC_5(CF_3)_4$
1.1418	$H_6-CH_2-CH(NH_3)-CO_2$	1.2375	$C_{10}H_8LiNO_3S \cdot 3H_2O$
1.1426	$C_7H_{12}N_2O_2 \cdot HBr$	1.2387	$C_{26}H_{20}Br_2P$
1.1427	$Fe(C_5H_4 \cdot COCH_3)_2$	1.2412	$C_{15}H_{14}O_7 \cdot H_2O$
1.1440	$C_{10}H_{22}N_4Ni(ClO_4)_2$	1.2414	$C_{19}H_{12}O_2$
1.1443	$H_6-CH_2-CH(NH_3)-CO_2$	1.2433	$Cu(ClCH_2COO)_2 \cdot 2.5H_2O$
1.1448	$C_5H_5NOICl$	1.2456	$AgAlCl_4 \cdot C_6H_6$
1.1465	$K_2Pd(CN)_4 \cdot H_2O$	1.2457	$C_{17}H_5OCl$
1.1476	$K(S \cdot CS \cdot OC_2H_5)$	1.2479	$C_8H_{16}N_2O_2$
1.1479	$C_{11}H_7NO$	1.2506	$(C_6H_5)_2V$
1.1479	$Sn_3(CH_3)_4Fe_4(CO)_{16}$	1.2507	$C_5H_5Fe(CO)_2HgCo(CO)_4$
1.1501	$Mn(N_2H_4)_2(H_2NNHC_6H_5)_2$	1.2528	$[(C_2H_5)_2NCS_2]_2Pb$
1.1508	$Rb(S \cdot CS \cdot OC_2H_5)$	1.2533	$C_4B_2O_2H_2$
1.1513	$Ni(C_2H_8N_2)_2(NCS)_2$	1.2537	$C_2H_5SHgCl$
1.1522	$(CH_4N_2O)_2 \cdot C_4H_6O_4$	1.2542	$C_4H_6Br_2S_2$
1.1566	$TiCl_2(C_4H_9)_2 \cdot C_4H_9OH$	1.2566	$Ni(C_2H_8N_2)_2Br_2$
1.1580	$C_{30}H_{38}O_4Cu$	1.2582	$C_8H_{13}O_3N$
1.1581	$C_{22}H_{28}N_2O_2Pd$	1.2609	$C_6H_8O_2 \cdot C_2I_2$
1.1586	$(C_3H_5PdCl)_2$	1.2624	$C_{16}H_8Cl_4$
1.1618	$Cr(C_6H_4N \cdot NC_6H_4)_2 \cdot C_5H_5NH$	1.2675	$Cd(C_7H_5O_3)_2 \cdot H_2O$
1.1637	$TiBr_2(C_4H_9)_2 \cdot C_4H_9OH$	1.2724	$C_4H_8O_2S_2$
1.1648	$Cr(C_5H_5)_2$	1.2732	$(CH_3)_3NCH_2COOHCl$
1.1665	$C_6H_6Cl_6$	1.2734	$[(CH_3)_2C_6H_5S]Cl_4$
1.1665	$NH_3 \cdot CH_2 \cdot CH_2 \cdot O \cdot P \cdot O_3H$	1.2756	$C_3H_7O \cdot C_6H_4 \cdot CH \cdot COOH$
1.1688	$C_{17}H_{14}BrN_5O_3$	1.2785	$C_9H_5Cl_6$
1.1696	$C_{14}H_{24}$	1.2807	$(C_6H_5)_2Hg$
1.1700	$C_5H_4NCH_2NH_2 \cdot 2HCl$	1.2821	$C_{15}H_{11}Cl_4S_2$
1.1716	$(PdCl(C_3H_5))_2$	1.2831	$C_6H_4ClNO_2$
1.1735	$C_4H_9COOH$	1.2833	$C_2H_5MgBr \cdot 2(C_4H_{10}O)$
1.1757	$(H_6OC \cdot C_6H_4)_2$	1.2850	$ClH_3NO(CH_2)_4NH_3Cl$
1.1783	$Cl \cdot C_6H_4 \cdot CHN(CH_3)_6$	1.2855	$C_{12}H_{10}BBR_2P$
1.1785	$Co(N_2H_4)_2(H_2NNHC_6H_5)_2$	1.2862	$C_{12}H_{10}BI_2P$
1.1803	$C_5H_{16}IN_5NiS$	1.2863	$FC_6H_4CONH_2$
1.1818	$B_{10}H_{12}[S(CH_3)_2]_2$	1.2880	$C_{12}H_{10} \cdot C_8H_8(NO_2)_2$
1.1821	$[(C_6H_{11})_3P]_2Ni(SCN)_2$	1.2889	$Rb_3Fe(CN)_6$
1.1847	$C_8[Th(NCS)_8] \cdot 2H_2O$	1.2904	$K_3Fe(CN)_6$
1.1916	$H_6OC \cdot C_6H_{10} \cdot COOH$	1.2928	$(H_2B[NH(CH_3)_2]_2)Cl$
1.1922	$NH_2 \cdot CO \cdot CO \cdot NH_4$	1.2931	$C_5H_5 \cdot (CF_3)_6C_6 \cdot Rh$
1.1930	$HgCl_2 \cdot C_6H_4(N(CH_3)_2)_2$	1.2939	$(C_5H_4 \cdot C_5H_4)Fe_2(C_5H_5)_2$
1.1930	$(C_5H_5)_2Be$	1.2943	$[C_5H_5 \cdot Mo(CO)_3]_2$
1.1932	$(C_5H_5)_2Fe$	1.2962	$(CH_3)_3NCH_2COOHBr$
1.1935	$C_6H_5 \cdot SO_2 \cdot CH_3$	1.2964	$C_6H_{10}O_4$
1.1938	$[C_6H_4(CH_3)_3]_2$	1.2964	$(C_6H_5)_2Hg$
1.1957	$AgSCN \cdot P(C_3H_7)_3$	1.2982	$(C_5H_5)Fe(C_5H_4COOC_6H_5)$
1.1961	$ZnI_2 \cdot 2NH_2CO(CH_3)_2$	1.2995	$C_{10}H_{12}O_6$
1.1981	$Sn(C_6H_4OC_2H_5)_4$	1.2996	$Zn(HCOO)_2 \cdot 2H_2O$
1.1992	$C_{10}H_{12}O_2$	1.3001	$NO_2C_6H_4OH$
1.1998	$Cu(C_{11}H_{12}N_2O)_5(ClO_4)_2$	1.3015	$(C_5H_5W)_2(CO)_6$
1.2034	$(CH_3CO)_2C_3H_2S_2Na \cdot 3H_2O$	1.3016	$C_8H_{17}NO$
1.2038	$C_{14}H_{10}Cr(CO)_3$	1.3017	$Th(C_5H_7O_2)_4$
1.2045	$C_2I_2 \cdot C_4H_8Se_2$	1.3034	$NO_2C_6H_4OH$
1.2068	$C_2H_2N_2S_3$	1.3037	$(CH_3)_3NCH_2CH_2OS_3$
1.2093	$(NC)_2C \cdot C(CN)_2$	1.3040	$C_3H_2N_2O_3$
1.2114	$C_2H_2N_2S_3$	1.3043	$Fe(HCOO)_2 \cdot 2H_2O$
1.2118	$C_6H_9 \cdot C_4H_8O_2$	1.3044	$U(C_5H_7O_2)_4$
1.2141	$C_2H_5COOH$	1.3045	$Ni(HCOO)_2 \cdot 2H_2O$
1.2143	$(CH_3C_6H_4)_3SbCl_2$	1.3056	$NO_2C_6H_4OH$
1.2158	$C_{14}H_8Br_2O$	1.3056	$C_{11}H_{15}N_5 \cdot HCl$
1.2160	$C_{11}H_{10}$	1.3063	$UO_2(C_5H_7O_2)_2 \cdot H_2O$
1.2161	$CH_3As(CN)_2$	1.3064	$C_3H_3N_6S_2$
1.2181	$C_5H_{10}N_2O_3$	1.3078	$Mg(HCOO)_2 \cdot 2H_2O$
1.2186	$Te(S_2COCH_3)_2$	1.3085	$Ce(C_5H_7O_2)_4$
1.2199	$[C_5H_4NCH(CH_3)NH(CH_2)_2N=CHC_5H_4N]CuBrClO_4$	1.3125	$NO_2C_6H_4OH$
1.2205	$C_4H_6Cl_2O_2$	1.3151	$(C_5H_4 \cdot C_5H_4)Fe_2(C_5H_5)_2$
1.2238	$C_{26}H_{20}Cl_6P$	1.3166	$C_{10}H_8$
1.2254	$(Cl-C_5H_4FeC_5H_4-)_2$	1.3169	$Mn(HCOO)_2 \cdot 2H_2O$

P<sub>2</sub>/c C<sub>2h</sub><sup>5</sup> No. 14 (continued)

## Organic (continued)

1.3187	C <sub>26</sub> H <sub>32</sub> Cl <sub>4</sub>	1.4430	[(C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> As] <sub>2</sub> (HgBr <sub>2</sub> ) <sub>3</sub>
1.3191	CdCl <sub>2</sub> (CH <sub>3</sub> C <sub>6</sub> NH <sub>2</sub> ) <sub>2</sub>	1.4441	ClH <sub>3</sub> N <sup>+</sup> CH <sub>2</sub> CH <sub>2</sub> NH <sub>3</sub> Cl
1.3200	C <sub>2</sub> I <sub>2</sub> •C <sub>4</sub> H <sub>8</sub> S <sub>2</sub>	1.4464	C <sub>20</sub> H <sub>28</sub> Cl
1.3210	HC-NH-NH-CH <sub>3</sub>	1.4487	C <sub>4</sub> H <sub>4</sub> N <sub>6</sub> Cl <sub>2</sub> H <sub>2</sub> Cl
1.3223	Zn(C <sub>2</sub> H <sub>5</sub> N <sub>3</sub> Cl <sub>2</sub> ) <sub>2</sub>	1.4489	Ca <sub>5</sub> Si <sub>2</sub> Cl <sub>7</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
1.3238	C <sub>12</sub> H <sub>22</sub> Br <sub>2</sub> N <sub>2</sub> Cl <sub>2</sub>	1.4495	NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub>
1.3243	Cd(HC <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> O	1.4531	[(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NCS <sub>2</sub> ] <sub>2</sub> Cu
1.3261	C <sub>30</sub> H <sub>20</sub> K <sub>2</sub> N <sub>4</sub> Cl <sub>4</sub>	1.4538	C <sub>9</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>6</sub> S <sub>8</sub> Te
1.3262	N <sub>6</sub> C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	1.4539	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>
1.3264	C <sub>5</sub> H <sub>4</sub> N <sup>+</sup> CH <sub>3</sub>	1.4590	Cu(C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> ) <sub>2</sub>
1.3270	(C <sub>12</sub> H <sub>9</sub> BrN <sub>2</sub> ) <sub>2</sub> Cu	1.4604	CuC <sub>2</sub> H <sub>4</sub> (C <sub>5</sub> H <sub>7</sub> N <sub>2</sub> ) <sub>2</sub>
1.3285	C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub>	1.4618	Ni(NH <sub>2</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> O
1.3287	Cu(HC <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> O	1.4623	Cl <sub>2</sub> C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>
1.3322	[C <sub>2</sub> H <sub>5</sub> S•Fe(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> ] <sub>2</sub>	1.4630	(C <sub>16</sub> H <sub>12</sub> ) <sub>2</sub>
1.3377	(B <sub>9</sub> C <sub>2</sub> H <sub>11</sub> )Re(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> CS	1.4633	[(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NCS <sub>2</sub> ] <sub>2</sub> Cu
1.3396	(CH <sub>3</sub> ) <sub>3</sub> N(CH <sub>2</sub> ) <sub>10</sub> N(CH <sub>3</sub> ) <sub>3</sub> •Br <sub>2</sub> •2H <sub>2</sub> O	1.4688	C <sub>3</sub> H <sub>7</sub> Cl•C <sub>6</sub> H <sub>4</sub> •CH <sub>2</sub> •CH•C <sub>6</sub> H <sub>5</sub>
1.3423	[Co(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> Br <sub>2</sub> ] <sub>2</sub> •Br•HBr•2H <sub>2</sub> O	1.4691	Zn(C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> ) <sub>2</sub>
1.3431	(C <sub>12</sub> H <sub>9</sub> BrN <sub>2</sub> ) <sub>2</sub> Cu	1.4708	C <sub>9</sub> H <sub>7</sub> ClS <sub>2</sub> •2H <sub>2</sub> O
1.3449	C <sub>30</sub> H <sub>14</sub> Cl <sub>2</sub>	1.4728	C <sub>2</sub> H <sub>2</sub> •GeI <sub>2</sub>
1.3462	CH <sub>3</sub> N <sub>5</sub> •H <sub>2</sub> O	1.4740	C <sub>24</sub> H <sub>18</sub>
1.3484	[(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> I][BF <sub>4</sub> ]	1.4746	C <sub>16</sub> H <sub>10</sub>
1.3488	C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> S <sub>2</sub>	1.4758	C <sub>16</sub> H <sub>16</sub>
1.3536	[Co(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> Cl <sub>2</sub> ] <sub>2</sub> •Cl•HCl•2H <sub>2</sub> O	1.4758	(NH <sub>4</sub> ) <sub>2</sub> C <sub>4</sub> H <sub>4</sub> Cl <sub>6</sub>
1.3537	NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> •CH <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	1.4759	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> Cl <sub>2</sub> •HBr
1.3549	C <sub>8</sub> H <sub>5</sub> N <sub>2</sub> Cl <sub>2</sub> Br	1.4762	KCu <sub>2</sub> (CN) <sub>3</sub> •H <sub>2</sub> O
1.3559	C <sub>20</sub> H <sub>28</sub> Cl	1.4785	(NCC) <sub>2</sub>
1.3630	Ni(C <sub>5</sub> H <sub>7</sub> Cl <sub>2</sub> ) <sub>2</sub> (C <sub>5</sub> H <sub>5</sub> N) <sub>2</sub>	1.4796	C <sub>8</sub> H <sub>4</sub> N <sub>6</sub> Cl <sub>2</sub> •C <sub>5</sub> H <sub>6</sub> N <sub>6</sub>
1.3632	C <sub>26</sub> H <sub>18</sub> I <sub>2</sub> CuN <sub>2</sub> Cl <sub>2</sub>	1.4841	KCu <sub>2</sub> (CN) <sub>3</sub> •H <sub>2</sub> O
1.3682	Fe(C <sub>6</sub> H <sub>7</sub> ) <sub>2</sub>	1.4853	Zn(C <sub>6</sub> H <sub>5</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
1.3718	C <sub>10</sub> H <sub>8</sub>	1.4854	[(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> As] <sub>2</sub> (HgI <sub>2</sub> ) <sub>2</sub>
1.3731	Li <sub>3</sub> C <sub>6</sub> H <sub>2</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> CH <sub>2</sub> Cl <sub>2</sub> •2H <sub>2</sub> O	1.4869	(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> Mn
1.3771	(C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>2</sub> (P <sub>6</sub> )-Cl <sub>2</sub> •C <sub>2</sub> H <sub>5</sub>	1.4873	C <sub>2</sub> H <sub>4</sub> •PtCl <sub>2</sub> •C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> (NH <sub>2</sub> ) <sub>2</sub> Cl
1.3780	C <sub>19</sub> H <sub>19</sub> N•HCNS	1.4877	Be <sub>4</sub> Cl <sub>2</sub> (CH <sub>3</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>6</sub>
1.3787	C <sub>5</sub> H <sub>4</sub> N <sup>+</sup> C <sub>3</sub> H <sub>2</sub> N <sup>-</sup>	1.4877	(TiCl <sub>4</sub> •CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> Cl) <sub>2</sub>
1.3795	C <sub>8</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub>	1.4887	C <sub>16</sub> H <sub>10</sub> •C <sub>10</sub> H <sub>2</sub> Cl <sub>6</sub>
1.3811	C <sub>28</sub> H <sub>16</sub> Cl <sub>2</sub>	1.4890	HgS <sub>4</sub> •3SC(NH <sub>2</sub> ) <sub>2</sub>
1.3839	C <sub>3</sub> N <sub>3</sub> (NH <sub>2</sub> ) <sub>3</sub>	1.4893	[(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NCS <sub>2</sub> ] <sub>2</sub> Cd
1.3857	[Co(C <sub>2</sub> H <sub>5</sub> (NH <sub>2</sub> ) <sub>2</sub> ) <sub>2</sub> (N <sub>2</sub> ) <sub>2</sub> NO <sub>3</sub>	1.4902	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>
1.3862	C <sub>14</sub> H <sub>10</sub> (CHCl) <sub>2</sub>	1.4908	C <sub>11</sub> H <sub>14</sub> N <sub>5</sub> Cl•HCl
1.3864	C <sub>14</sub> H <sub>13</sub> Br <sub>2</sub>	1.4922	C <sub>3</sub> H <sub>5</sub> Cl•C <sub>6</sub> H <sub>4</sub> •CH <sub>2</sub> •CH•C <sub>6</sub> H <sub>5</sub>
1.3895	C <sub>18</sub> H <sub>20</sub>	1.4941	Cd(S <sub>2</sub> CN(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ) <sub>2</sub>
1.3917	((CH <sub>3</sub> ) <sub>4</sub> Si <sub>2</sub> Cl <sub>3</sub> ) <sub>2</sub> Al <sub>3</sub> Br <sub>5</sub>	1.4969	C <sub>12</sub> H <sub>24</sub> Cl <sub>2</sub> N <sub>8</sub> S <sub>8</sub> Te
1.3921	[Cr(C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> ) <sub>2</sub> Cl <sub>2</sub> ] <sub>2</sub> •Cl•HCl•2H <sub>2</sub> O	1.4970	(C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>3</sub>
1.3933	C <sub>10</sub> H <sub>7</sub> Cl	1.4981	C <sub>11</sub> H <sub>14</sub> ClN <sub>5</sub> •HBr
1.3943	[(CH <sub>3</sub> ) <sub>3</sub> Pt(C <sub>3</sub> H <sub>7</sub> Cl•CH <sub>2</sub> •C <sub>6</sub> H <sub>5</sub> )] <sub>2</sub>	1.4985	C <sub>3</sub> H <sub>5</sub> N <sub>11</sub> Ni <sub>6</sub> S <sub>3</sub>
1.3946	C <sub>10</sub> H <sub>8</sub>	1.5008	Cl(NH <sub>2</sub> )N(CH <sub>3</sub> ) <sub>2</sub>
1.3949	Fe(C <sub>5</sub> H <sub>4</sub> S <sub>2</sub> Cl) <sub>2</sub>	1.5032	Ag <sub>2</sub> C <sub>2</sub> Cl <sub>4</sub>
1.3952	C <sub>8</sub> H <sub>10</sub> Br <sub>2</sub> Cl <sub>2</sub>	1.5039	C <sub>26</sub> H <sub>22</sub> N <sub>2</sub> Cl <sub>2</sub>
1.3953	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> AsCl	1.5065	B <sub>20</sub> H <sub>16</sub> (NCCH <sub>3</sub> ) <sub>2</sub> •CH <sub>3</sub> CN
1.3970	Ni(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> Cl) <sub>2</sub> •2H <sub>2</sub> O	1.5070	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> S
1.3991	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> AsI	1.5089	(CH <sub>4</sub> N <sub>2</sub> ) <sub>2</sub> •C <sub>6</sub> H <sub>10</sub> Cl <sub>4</sub>
1.4003	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>	1.5090	C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub>
1.4010	C <sub>8</sub> H <sub>4</sub> Cl <sub>4</sub>	1.5096	C <sub>8</sub> H <sub>16</sub> N <sub>6</sub> S <sub>2</sub>
1.4047	Fe(C <sub>5</sub> H <sub>4</sub> Cl) <sub>2</sub> [C(CH <sub>3</sub> ) <sub>2</sub> •C <sub>5</sub> H <sub>4</sub> ]	1.5103	C <sub>7</sub> H <sub>16</sub> ClN <sub>5</sub> S
1.4053	Nd(CH <sub>2</sub> Cl•CH <sub>2</sub> Cl•CH <sub>3</sub> ) <sub>3</sub>	1.5123	CuCl <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> (N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>2</sub>
1.4054	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> BrAs	1.5131	C <sub>6</sub> Cl <sub>4</sub> Cl <sub>2</sub>
1.4105	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> P=C•C•Cl	1.5164	CH <sub>3</sub> Cl•C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub>
1.4209	ClCH <sub>2</sub> CH <sub>2</sub> Cl	1.5185	C <sub>21</sub> H <sub>29</sub> Br <sub>3</sub> S
1.4253	[Se(CH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub>	1.5195	SSb(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub>
1.4256	Ni[ClC <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> N(CH <sub>2</sub> ) <sub>3</sub> ] <sub>2</sub> NCH <sub>3</sub>	1.5248	C <sub>13</sub> H <sub>22</sub> Cl <sub>2</sub> N <sub>2</sub> S•HCl
1.4263	CoCl <sub>2</sub> •4CH <sub>3</sub> OH	1.5265	(C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> ) <sub>2</sub> Cu
1.4275	C <sub>6</sub> H <sub>5</sub> (NH <sub>2</sub> CSNH <sub>2</sub> )TeCl	1.5280	N <sub>6</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>
1.4286	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	1.5287	Cu(NCS) <sub>3</sub> [(NH <sub>2</sub> ) <sub>2</sub> CS]
1.4295	(C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>2</sub> (P <sub>6</sub> )SC <sub>2</sub> H <sub>5</sub>	1.5303	CuCl <sub>2</sub> •C <sub>2</sub> H <sub>4</sub> (C <sub>2</sub> H <sub>6</sub> N <sub>5</sub> ) <sub>2</sub> •H <sub>2</sub> O
1.4305	C <sub>6</sub> H <sub>2</sub> (C <sub>2</sub> H <sub>3</sub> ) <sub>2</sub>	1.5312	C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub>
1.4315	C <sub>6</sub> H <sub>5</sub> (NH <sub>2</sub> CSNH <sub>2</sub> )TeBr	1.5347	C <sub>42</sub> H <sub>28</sub>
1.4330	C <sub>4</sub> H <sub>8</sub> S <sub>2</sub>	1.5350	C <sub>8</sub> H <sub>8</sub> Br <sub>3</sub>
1.4356	C <sub>4</sub> H <sub>8</sub> S <sub>2</sub>	1.5363	C <sub>6</sub> H <sub>8</sub> Br <sub>4</sub>
1.4357	K <sub>2</sub> Ce(CH <sub>3</sub> Cl) <sub>5</sub> •H <sub>2</sub> O	1.5375	C <sub>7</sub> H <sub>7</sub> Cl <sub>2</sub> OH
1.4371	C <sub>26</sub> H <sub>30</sub> Cl <sub>5</sub>	1.5378	(CH <sub>3</sub> NHCH <sub>2</sub> CH <sub>2</sub> NHCH <sub>3</sub> ) <sub>2</sub> Cu(N <sub>2</sub> ) <sub>3</sub>
1.4389	Zn[S <sub>2</sub> CN(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ] <sub>2</sub>	1.5385	C <sub>18</sub> H <sub>18</sub>
1.4400	C <sub>6</sub> H <sub>5</sub> •CH <sub>2</sub> •CH <sub>2</sub> •CH <sub>2</sub> •CH <sub>2</sub> •C <sub>6</sub> H <sub>5</sub>	1.5427	CF <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> NH <sub>4</sub>
1.4400	2(CH <sub>3</sub> OH)•Br <sub>2</sub>	1.5488	C <sub>16</sub> H <sub>10</sub> •C <sub>10</sub> H <sub>2</sub> Cl <sub>6</sub>
1.4422	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> Cl <sub>2</sub>	1.5497	SP(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub>



P2<sub>1</sub>/c C<sub>2h</sub><sup>5</sup> No. 14 (continued)

## Organic (continued)

1.5516	Se <sub>2</sub> (S <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	1.6727	Ni(C <sub>14</sub> H <sub>10</sub> S <sub>2</sub> ) <sub>2</sub>
1.5563	KSeCN	1.6789	C <sub>5</sub> H <sub>5</sub> Mn(C <sub>6</sub> ) <sub>3</sub>
1.5569	C <sub>9</sub> H <sub>12</sub> N <sub>4</sub> Cl <sub>3</sub>	1.6795	C <sub>8</sub> H <sub>2</sub> Cl <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>
1.5571	C <sub>6</sub> H <sub>3</sub> (OH) <sub>2</sub> NH <sub>2</sub> HCl	1.6809	C <sub>22</sub> H <sub>16</sub>
1.5578	Sc(HCO <sub>2</sub> ) <sub>3</sub>	1.6882	C <sub>6</sub> H <sub>5</sub> •C <sub>6</sub> H <sub>5</sub>
1.5588	(C <sub>9</sub> H <sub>12</sub> Cl <sub>4</sub> ) <sub>2</sub>	1.6886	NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> (CH <sub>2</sub> ) <sub>2</sub> CH <sub>3</sub>
1.5594	C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> Cl <sub>2</sub>	1.6906	CHN <sub>4</sub> NHN <sub>2</sub>
1.5599	C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub> Br <sub>2</sub>	1.6960	C <sub>5</sub> H <sub>8</sub> N <sub>4</sub> S
1.5613	C <sub>11</sub> H <sub>9</sub> N <sub>2</sub> Cl <sub>3</sub>	1.6962	Ni[C <sub>6</sub> H <sub>4</sub> (As[CH <sub>3</sub> ] <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> I <sub>2</sub>
1.5614	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> S <sub>2</sub>	1.6964	Mg(C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> S) <sub>2</sub> •10H <sub>2</sub> O
1.5628	C <sub>18</sub> H <sub>19</sub> Cl <sub>3</sub>	1.6966	K <sub>2</sub> Ni(CN) <sub>4</sub>
1.5638	C <sub>14</sub> H <sub>10</sub>	1.7014	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>
1.5640	C <sub>6</sub> H <sub>2</sub> Cl <sub>2</sub> Cl <sub>4</sub>	1.7045	(PCF <sub>3</sub> ) <sub>5</sub>
1.5645	C <sub>14</sub> H <sub>10</sub>	1.7052	C <sub>14</sub> H <sub>14</sub> As <sub>2</sub> •2I
1.5650	Te(C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> S) <sub>2</sub> (S <sub>2</sub> C <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	1.7057	C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> Ni <sub>2</sub>
1.5670	C <sub>7</sub> H <sub>8</sub> SSe	1.7102	C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> •H <sub>2</sub> S <sub>2</sub>
1.5678	C <sub>28</sub> H <sub>24</sub> N <sub>4</sub>	1.7123	(CH <sub>3</sub> ) <sub>2</sub> S <sub>2</sub>
1.5704	(CH <sub>2</sub> ) <sub>6</sub>	1.7170	C <sub>7</sub> H <sub>5</sub> N <sub>2</sub> S
1.5719	C <sub>4</sub> H <sub>2</sub> Br <sub>6</sub>	1.7174	Pt[C <sub>6</sub> H <sub>4</sub> (As[CH <sub>3</sub> ] <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> I <sub>2</sub>
1.5744	H <sub>2</sub> C(CH <sub>2</sub> ) <sub>5</sub> C <sub>6</sub> H <sub>5</sub>	1.7226	(H <sub>2</sub> C <sub>2</sub> N <sub>2</sub> Cl <sub>2</sub> ) <sub>2</sub> Ni
1.5770	Cu[S <sub>2</sub> CN(CH <sub>2</sub> ) <sub>6</sub> ] <sub>2</sub>	1.7273	Pd[C <sub>6</sub> H <sub>4</sub> (As[CH <sub>3</sub> ] <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> I <sub>2</sub>
1.5772	ClC <sub>6</sub> H <sub>4</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> PS	1.7301	H <sub>2</sub> NCNHNH <sub>2</sub>
1.5775	Fe(S <sub>2</sub> CN(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ) <sub>2</sub> Cl	1.7306	Fe(CH <sub>2</sub> OH•C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub>
1.5787	[Cu(NH <sub>2</sub> CSNH <sub>2</sub> ) <sub>3</sub> ] <sub>2</sub> S <sub>2</sub> •2H <sub>2</sub> O	1.7306	NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> (CH <sub>2</sub> ) <sub>2</sub> CH <sub>3</sub>
1.5805	((C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> AsC <sub>6</sub> H <sub>4</sub> ) <sub>3</sub> As•HgBr <sub>2</sub> •CH <sub>2</sub> Cl <sub>2</sub>	1.7311	C <sub>6</sub> H <sub>3</sub> BrN <sub>2</sub> Cl <sub>2</sub>
1.5817	C <sub>7</sub> H <sub>10</sub> Cl <sub>4</sub> S <sub>2</sub>	1.7322	Cu(C <sub>10</sub> H <sub>9</sub> Cl <sub>2</sub> ) <sub>2</sub>
1.5825	C <sub>14</sub> H <sub>13</sub> BrN <sub>4</sub> Cl <sub>3</sub> •H <sub>2</sub> O	1.7333	HgCl <sub>2</sub> •2(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> P <sub>2</sub>
1.5826	C <sub>8</sub> H <sub>8</sub> Cl <sub>4</sub>	1.7350	C <sub>6</sub> Cl <sub>4</sub> Cl <sub>2</sub> •C <sub>6</sub> (CH <sub>3</sub> ) <sub>6</sub>
1.5826	C <sub>10</sub> H <sub>4</sub> Br <sub>2</sub> I <sub>2</sub>	1.7353	CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub>
1.5864	Cu[(CH <sub>2</sub> ) <sub>4</sub> NH(NH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> Cl <sub>2</sub> •H <sub>2</sub> O	1.7376	Mg <sub>2</sub> U <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> •18H <sub>2</sub> O
1.5873	K <sub>3</sub> [Cr(Cl <sub>2</sub> ) <sub>2</sub> (CN) <sub>3</sub> ]	1.7391	HgCl <sub>2</sub> •2[(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> As <sub>2</sub> ]
1.5898	RuCl <sub>2</sub> (C <sub>12</sub> H <sub>18</sub> )	1.7407	Mg <sub>2</sub> U <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> •18H <sub>2</sub> O
1.5902	C <sub>10</sub> H <sub>10</sub> NNaCl <sub>2</sub> •1.5H <sub>2</sub> O	1.7416	C <sub>22</sub> H <sub>18</sub>
1.5905	C <sub>6</sub> H <sub>8</sub> Cl <sub>4</sub>	1.7423	CuC <sub>20</sub> H <sub>18</sub> Cl <sub>4</sub>
1.5911	CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> OH	1.7429	MoC <sub>7</sub> H <sub>6</sub> (C <sub>6</sub> ) <sub>3</sub>
1.5948	C <sub>7</sub> H <sub>8</sub> Cl <sub>2</sub>	1.7449	C <sub>18</sub> Cl <sub>3</sub> H <sub>19</sub>
1.5967	(C <sub>6</sub> H <sub>5</sub> CO) <sub>3</sub> CN•NC <sub>6</sub> H <sub>5</sub>	1.7450	C <sub>4</sub> H <sub>9</sub> OLi•C <sub>4</sub> H <sub>9</sub> Li
1.5981	C <sub>2</sub> H <sub>2</sub> •GeCl <sub>2</sub>	1.7475	(C <sub>6</sub> H <sub>5</sub> C•C•) <sub>2</sub> Hg
1.6005	C <sub>21</sub> H <sub>16</sub>	1.7527	(CH <sub>3</sub> ) <sub>3</sub> Pt(C <sub>5</sub> H <sub>7</sub> Cl <sub>2</sub> )C <sub>10</sub> N <sub>2</sub> H <sub>8</sub>
1.6043	Pt(NH <sub>3</sub> ) <sub>2</sub> (SCN) <sub>2</sub>	1.7532	Zn[NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> ] <sub>2</sub> Cl <sub>2</sub>
1.6044	Ni[(CH <sub>2</sub> ) <sub>4</sub> NH(NH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> Cl <sub>2</sub> •H <sub>2</sub> O	1.7534	P <sub>2</sub> (CH <sub>3</sub> ) <sub>4</sub> •2BH <sub>3</sub>
1.6061	(C <sub>8</sub> H <sub>14</sub> ) <sub>2</sub> Cl <sub>4</sub>	1.7542	AsC <sub>6</sub> H <sub>5</sub> [SCSN(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ] <sub>2</sub>
1.6140	C <sub>7</sub> H <sub>8</sub> Se <sub>2</sub>	1.7546	Cu(C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> ) <sub>2</sub>
1.6142	C <sub>26</sub> H <sub>22</sub> N <sub>2</sub> Cl <sub>2</sub>	1.7548	CaC <sub>2</sub>
1.6142	Co(NH <sub>2</sub> CS <sub>2</sub> ) <sub>3</sub>	1.7562	Li <sub>2</sub> C <sub>2</sub> Cl <sub>4</sub>
1.6147	C <sub>5</sub> H <sub>5</sub> Rh(C <sub>6</sub> )(C <sub>2</sub> F <sub>5</sub> ) <sub>1</sub>	1.7639	C <sub>19</sub> H <sub>19</sub> N(OH) <sub>2</sub>
1.6165	CH <sub>2</sub> :CH•C <sub>6</sub> H <sub>4</sub> •NH <sub>2</sub>	1.7663	C <sub>6</sub> H <sub>3</sub> ClN <sub>2</sub> Cl <sub>2</sub>
1.6236	Cl <sub>2</sub> NiC <sub>10</sub> H <sub>24</sub> N <sub>4</sub>	1.7692	Cu <sub>3</sub> (OH) <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
1.6236	C <sub>4</sub> H <sub>16</sub> N <sub>6</sub> Ni <sub>2</sub> Cl <sub>4</sub>	1.7709	C <sub>14</sub> H <sub>8</sub> BrN <sub>5</sub> Cl <sub>2</sub> •0.5C <sub>7</sub> H <sub>8</sub>
1.6239	N <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> •C <sub>6</sub> H <sub>5</sub>	1.7723	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> Cl <sub>3</sub>
1.6279	Cl(N <sub>2</sub> ) <sub>2</sub> CH <sub>3</sub>	1.7734	(C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> ) <sub>2</sub> Cu
1.6284	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> Cl <sub>3</sub>	1.7798	C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> Ni <sub>2</sub>
1.6348	C <sub>6</sub> H <sub>7</sub> N <sub>5</sub> OHBr	1.7808	C <sub>30</sub> H <sub>20</sub> Cl <sub>2</sub>
1.6385	(OCNH <sub>2</sub> CH <sub>2</sub> ) <sub>6</sub> NH•C <sub>6</sub> H <sub>4</sub> (CH <sub>2</sub> ) <sub>4</sub> •Cl <sub>2</sub>	1.7835	C <sub>24</sub> H <sub>18</sub>
1.6390	C <sub>9</sub> H <sub>11</sub> N <sub>3</sub> Cl <sub>4</sub>	1.7874	[(C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> P] <sub>2</sub> (HgBr <sub>2</sub> ) <sub>2</sub>
1.6392	(C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> Cl) <sub>2</sub> Ni(C <sub>6</sub> ) <sub>2</sub>	1.7928	C <sub>12</sub> H <sub>10</sub> Cl <sub>2</sub>
1.6420	(C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> Cl) <sub>2</sub> Pd(C <sub>6</sub> ) <sub>2</sub>	1.7939	Cu <sub>2</sub> Cl <sub>2</sub> N <sub>4</sub> C <sub>16</sub> H <sub>16</sub> Cl <sub>2</sub> •2H <sub>2</sub> O
1.6422	Ru(S <sub>2</sub> CN(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ) <sub>3</sub>	1.7949	C <sub>20</sub> H <sub>12</sub>
1.6487	C <sub>6</sub> H <sub>2</sub> NH <sub>2</sub> (N <sub>2</sub> ) <sub>3</sub>	1.7960	C <sub>12</sub> H <sub>17</sub> N <sub>3</sub> Cl <sub>3</sub>
1.6516	C <sub>10</sub> H <sub>6</sub> Br <sub>2</sub>	1.7977	C <sub>12</sub> H <sub>16</sub> Cl <sub>2</sub>
1.6536	C <sub>10</sub> H <sub>26</sub> N <sub>4</sub> •4HCl	1.7991	(H <sub>2</sub> C•C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> CS•H <sub>2</sub> O
1.6542	AlCl <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> N <sub>2</sub>	1.8000	Cr(C <sub>6</sub> H <sub>4</sub> ) <sub>4</sub> •C <sub>6</sub> H <sub>4</sub> [As(CH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub>
1.6550	C <sub>3</sub> H <sub>4</sub> NS(CH <sub>3</sub> ):C <sub>3</sub> N <sub>2</sub> S <sub>2</sub> •C <sub>2</sub> H <sub>5</sub>	1.8053	C <sub>6</sub> H <sub>6</sub>
1.6563	(CH <sub>3</sub> ) <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	1.8056	NH <sub>4</sub> CNS
1.6566	Ni(C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> ) <sub>2</sub>	1.8065	Br <sub>2</sub> C <sub>6</sub> H <sub>2</sub> Cl <sub>2</sub>
1.6600	Hg[SC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>4</sub> Cl <sub>2</sub>	1.8069	C <sub>14</sub> H <sub>24</sub> Cl <sub>4</sub>
1.6604	[C <sub>13</sub> H <sub>12</sub> Cl <sub>2</sub> ]	1.8075	NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> (CH <sub>2</sub> ) <sub>3</sub> CH <sub>3</sub>
1.6621	CH <sub>2</sub> =C(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> PF <sub>3</sub> H(C <sub>6</sub> H <sub>11</sub> NH <sub>3</sub> )	1.8080	C <sub>10</sub> H <sub>4</sub> Cl <sub>2</sub> (OH) <sub>2</sub>
1.6624	K(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> S <sub>2</sub>	1.8104	(C <sub>6</sub> H <sub>4</sub> CH:NC <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> Cu
1.6649	C <sub>16</sub> H <sub>15</sub> Br <sub>2</sub> N <sub>3</sub> Cl <sub>2</sub> Si•C <sub>3</sub> H <sub>6</sub> Cl	1.8125	C <sub>6</sub> H <sub>3</sub> (N <sub>2</sub> ) <sub>2</sub> Cl <sub>2</sub> •H <sub>2</sub> O•C <sub>10</sub> H <sub>6</sub> BrNH <sub>2</sub>
1.6707	C <sub>5</sub> H <sub>5</sub> Fe(C <sub>6</sub> ) <sub>2</sub> C <sub>5</sub> H <sub>5</sub>	1.8190	C <sub>8</sub> H <sub>8</sub> ClN <sub>2</sub>
1.6725	C <sub>10</sub> H <sub>21</sub> S <sub>2</sub> Na•0.5H <sub>2</sub> O	1.8197	C <sub>4</sub> H <sub>4</sub> N <sub>1</sub> S <sub>4</sub>
1.6726	ReC <sub>13</sub> H <sub>19</sub>	1.8208	C <sub>40</sub> H <sub>20</sub>

P2<sub>1</sub>/c C<sub>2h</sub><sup>5</sup> No. 14 (continued)

## Organic (continued)

1.8240	(C <sub>7</sub> H <sub>5</sub> ) <sub>2</sub> Cu	1.9617	Ni(C <sub>5</sub> H <sub>11</sub> ) <sub>2</sub> [P(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ] <sub>2</sub>
1.8246	C <sub>20</sub> H <sub>14</sub> N <sub>4</sub>	1.9625	H <sub>6</sub> CC(CH <sub>2</sub> ) <sub>7</sub> CC <sub>6</sub> H <sub>5</sub>
1.8276	Pd(σ-C <sub>6</sub> H <sub>4</sub> C:N <sup>+</sup> C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub>	1.9632	C <sub>6</sub> H <sub>4</sub> ClN <sub>2</sub>
1.8304	NH <sub>2</sub> C <sup>+</sup> (CH <sub>2</sub> ) <sub>8</sub> C <sup>-</sup> NH <sub>2</sub>	1.9648	Zn(C <sub>5</sub> H <sub>4</sub> N <sup>+</sup> C <sub>5</sub> H <sub>3</sub> N <sup>+</sup> C <sub>5</sub> H <sub>4</sub> N)Cl <sub>2</sub>
1.8307	(CH <sub>3</sub> ) <sub>2</sub> TeCl <sub>2</sub>	1.9664	C <sub>12</sub> H <sub>10</sub> <sup>+</sup>
1.8320	C <sub>20</sub> H <sub>17</sub> Cl <sub>3</sub> <sup>+</sup>	1.9677	C <sub>2</sub> Na <sub>2</sub> <sup>+</sup>
1.8355	[NiN(CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>3</sub> ] <sub>3</sub> S <sup>+</sup> <sub>4</sub> •7H <sub>2</sub> O	1.9678	(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> C <sub>4</sub> H <sub>2</sub> Fe(C <sup>+</sup> ) <sub>4</sub>
1.8371	(NaC <sub>2</sub> H <sub>5</sub> OC <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> H <sub>2</sub> Be <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub>	1.9694	Cu(NH <sub>2</sub> •C <sub>5</sub> H <sub>8</sub> •C <sup>+</sup> ) <sub>2</sub>
1.8380	(σC <sub>6</sub> H <sub>4</sub> CH:NC <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> Ni	1.9715	Ca(C <sub>10</sub> H <sub>8</sub> N <sub>3</sub> S) <sub>2</sub> •8H <sub>2</sub> O
1.8396	C <sub>4</sub> H <sub>7</sub> <sup>+</sup> N <sup>+</sup> HCl•0.5H <sub>2</sub> O	1.9717	RbH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> <sup>+</sup>
1.8457	C <sub>14</sub> H <sub>14</sub> <sup>+</sup> N <sub>2</sub>	1.9723	C <sub>3</sub> H <sub>5</sub> C <sup>+</sup> NH <sub>2</sub>
1.8469	C <sub>2</sub> H <sub>11</sub> B <sub>10</sub> I	1.9731	Co(C <sub>4</sub> H <sub>7</sub> N <sub>2</sub> <sup>+</sup> ) <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub> N <sup>+</sup>
1.8473	Cl <sub>2</sub> C <sub>6</sub> H <sub>2</sub> <sup>+</sup>	1.9781	Co(C <sub>15</sub> H <sub>11</sub> N <sub>3</sub> )Cl <sub>2</sub>
1.8477	C <sub>6</sub> H <sub>2</sub> Cl(N <sup>+</sup> ) <sub>3</sub>	1.9785	CH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> •C <sup>+</sup>
1.8479	C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> <sup>+</sup> Rb <sub>2</sub> •2H <sub>2</sub> O	1.9790	CuCl <sub>2</sub> (C <sub>5</sub> H <sub>5</sub> N) <sub>2</sub>
1.8516	C <sub>10</sub> H <sub>4</sub> <sup>+</sup> (OH) <sub>2</sub>	1.9816	Cu(C <sub>15</sub> H <sub>11</sub> N <sub>3</sub> )Cl <sub>2</sub>
1.8528	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> •HCl•H <sub>2</sub> O	1.9818	Mn(C <sub>15</sub> H <sub>11</sub> N <sub>3</sub> )Cl <sub>2</sub>
1.8536	(C <sub>10</sub> H <sub>8</sub> N <sup>+</sup> S)NH <sub>4</sub> •H <sub>2</sub> O	1.9834	Cu(C <sub>5</sub> H <sub>5</sub> N) <sub>2</sub> Cl <sub>2</sub>
1.8537	2(CH <sub>3</sub> C <sup>+</sup> NHCH <sub>3</sub> )•NaCl <sup>+</sup>	1.9842	(C <sup>+</sup> ) <sub>2</sub> •2D <sub>2</sub> <sup>+</sup>
1.8539	C <sub>6</sub> H <sub>5</sub> SC <sub>6</sub> H <sub>3</sub> CH <sub>3</sub> N <sup>+</sup>	1.9864	C <sub>16</sub> H <sub>10</sub> •C <sub>2</sub> (CN) <sub>4</sub>
1.8566	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> S•HCl	1.9870	HGa(H <sub>2</sub> O)(σC•CH <sub>2</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(CH <sub>2</sub> C <sup>+</sup> ) <sub>2</sub>
1.8567	C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> ) <sub>2</sub>	1.9886	Mn(C <sub>5</sub> H <sub>5</sub> N) <sub>2</sub> Cl <sub>2</sub>
1.8594	(NH <sub>2</sub> CH <sub>2</sub> C <sup>+</sup> ) <sub>2</sub> HNO <sub>3</sub>	1.9912	C <sub>18</sub> H <sub>14</sub> Na <sub>2</sub> <sup>+</sup> •0.5C <sub>3</sub> H <sub>7</sub> O
1.8650	C <sub>12</sub> H <sub>8</sub>	1.9912	C <sub>16</sub> H <sub>23</sub> N <sup>+</sup> •HBr
1.8688	C <sub>10</sub> H <sub>10</sub> N <sub>2</sub>	1.9927	C <sub>16</sub> H <sub>16</sub>
1.8728	[(CH <sub>3</sub> ) <sub>2</sub> NCS] <sub>2</sub> S	1.9931	C <sub>16</sub> H <sub>10</sub> N <sub>2</sub> <sup>+</sup>
1.8732	C <sub>10</sub> H <sub>6</sub> (CH <sub>3</sub> ) <sub>2</sub>	1.9940	HFe(H <sub>2</sub> O)(σC•CH <sub>2</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(CH <sub>2</sub> C <sup>+</sup> ) <sub>2</sub>
1.8837	Ag(C <sub>8</sub> H <sub>2</sub> )N <sup>+</sup>	1.9942	CH <sub>2</sub> Cl•C <sup>+</sup> NH <sub>2</sub>
1.8843	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> <sup>+</sup>	1.9976	Cd(C <sub>5</sub> H <sub>4</sub> N <sup>+</sup> C <sub>5</sub> H <sub>3</sub> N <sup>+</sup> C <sub>5</sub> H <sub>4</sub> N)Cl <sub>2</sub>
1.8876	[Ru(C <sub>2</sub> H <sub>7</sub> N <sub>5</sub> ) <sub>3</sub> ] <sub>2</sub> (Se <sub>4</sub> ) <sub>3</sub> •7H <sub>2</sub> O	1.9983	CH <sub>2</sub> Cl•C <sup>+</sup> NH <sub>2</sub>
1.8890	C <sub>10</sub> H <sub>4</sub> <sup>+</sup> (OH) <sub>2</sub>	2.0000	HCr(H <sub>2</sub> O)(σC•CH <sub>2</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(CH <sub>2</sub> C <sup>+</sup> ) <sub>2</sub>
1.8898	(N <sup>+</sup> ) <sub>3</sub> C <sub>6</sub> H <sub>2</sub> OC <sub>2</sub> H <sub>5</sub> •Cs <sup>+</sup> OC <sub>2</sub> H <sub>5</sub>	2.0000	(C <sub>6</sub> H <sub>2</sub> (N <sup>+</sup> ) <sub>3</sub> )NH <sup>+</sup> C <sub>6</sub> H <sub>5</sub>
1.8908	C <sub>6</sub> H <sub>2</sub> (CH <sub>3</sub> ) <sub>4</sub>	2.0000	CH <sub>2</sub> Br•C <sup>+</sup> NH <sub>2</sub>
1.8929	C <sub>18</sub> H <sub>19</sub> Cl <sub>3</sub>	2.0000	H <sub>6</sub> CC(CH <sub>2</sub> ) <sub>6</sub> C <sup>+</sup>
1.8946	C <sub>4</sub> H <sub>3</sub> N <sub>3</sub> <sup>+</sup>	2.0013	Zn[NH <sub>2</sub> C <sup>+</sup> NHNH <sub>2</sub> ] <sub>2</sub> Cl <sub>2</sub>
1.8958	(C <sub>5</sub> H <sub>4</sub> N) <sub>2</sub>	2.0073	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> Cl <sub>2</sub>
1.8969	C <sub>14</sub> H <sub>14</sub>	2.0093	C <sub>14</sub> H <sub>20</sub> Cl <sub>2</sub>
1.9035	(C <sub>5</sub> H <sub>4</sub> N) <sub>2</sub>	2.0122	C <sub>3</sub> H <sub>7</sub> •C <sub>6</sub> H <sub>4</sub> •CH:CH•C <sup>+</sup>
1.9054	C <sub>6</sub> H <sub>13</sub> N <sup>+</sup> •HBr	2.0128	H <sub>6</sub> CC•CH <sub>2</sub> •CH:CH•CH <sub>2</sub> C <sup>+</sup>
1.9069	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> (CH <sub>2</sub> ) <sub>2</sub>	2.0187	(C <sub>11</sub> H <sub>12</sub> N <sup>+</sup> ) <sub>2</sub> Ni
1.9091	C <sub>12</sub> H <sub>25</sub> Se <sub>3</sub> Na•0.5H <sub>2</sub> O	2.0210	(C <sub>6</sub> H <sub>4</sub> CH <sup>+</sup> NC <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> Ni
1.9091	C <sub>10</sub> H <sub>15</sub> <sup>+</sup> N•HCl	2.0233	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> <sup>+</sup>
1.9103	(C <sub>5</sub> H <sub>4</sub> N) <sub>2</sub>	2.0305	Cu(C <sub>11</sub> H <sub>11</sub> <sup>+</sup> ) <sub>2</sub>
1.9109	Fe(C <sup>+</sup> ) <sub>2</sub> C <sub>5</sub> H <sub>4</sub> CH <sub>2</sub> Fe(C <sup>+</sup> ) <sub>4</sub>	2.0312	C <sub>14</sub> H <sub>14</sub> Cl <sub>6</sub> Sb <sub>2</sub>
1.9126	AgBF <sub>4</sub> •3C <sub>10</sub> H <sub>10</sub>	2.0323	N <sup>+</sup> <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> •NH <sub>2</sub>
1.9167	C <sub>20</sub> H <sub>12</sub>	2.0345	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>
1.9169	CN(C <sub>5</sub> H <sub>4</sub> N) <sup>+</sup>	2.0351	U <sup>+</sup> <sub>2</sub> •H <sub>2</sub> N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> •(S <sub>2</sub> CN(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ) <sub>3</sub>
1.9170	C <sub>20</sub> H <sub>12</sub> •C <sub>2</sub> (CN) <sub>4</sub>	2.0373	C <sub>10</sub> H <sub>12</sub> <sup>+</sup>
1.9184	C <sub>10</sub> H <sub>4</sub> <sup>+</sup> (OH) <sub>2</sub>	2.0387	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> <sup>+</sup>
1.9192	C <sub>12</sub> H <sub>9</sub> I	2.0389	Te(S <sub>2</sub> <sup>+</sup> <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
1.9211	C <sub>5</sub> H <sub>3</sub> N(C <sup>+</sup> ) <sub>2</sub> •HCl	2.0397	C <sub>10</sub> H <sub>7</sub> •C <sub>6</sub> H <sub>5</sub>
1.9227	ClBrC <sub>6</sub> H <sub>2</sub> <sup>+</sup>	2.0409	C <sub>20</sub> H <sub>12</sub> •C <sub>10</sub> H <sub>2</sub> <sup>+</sup>
1.9229	(C <sub>6</sub> H <sub>5</sub> OH) <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> <sup>+</sup>	2.0439	Cd(C <sub>5</sub> H <sub>4</sub> N) <sub>2</sub> Cl <sub>2</sub>
1.9254	C <sub>6</sub> H <sub>6</sub> •C <sub>10</sub> H <sub>2</sub> <sup>+</sup>	2.0535	C <sub>12</sub> H <sub>26</sub> N <sub>2</sub> <sup>+</sup>
1.9263	C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> <sup>+</sup>	2.0537	C <sub>8</sub> H <sub>12</sub> NiCl <sub>2</sub>
1.9283	C <sub>10</sub> H <sub>15</sub> <sup>+</sup> N•HBr	2.0541	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub> •C <sub>6</sub> H <sub>2</sub> (N <sup>+</sup> ) <sub>3</sub> OH
1.9329	C <sub>17</sub> H <sub>13</sub> N	2.0555	C <sub>3</sub> Cl <sub>6</sub>
1.9350	C <sub>16</sub> H <sub>23</sub> N <sup>+</sup> •HCl	2.0575	C <sub>20</sub> H <sub>28</sub> <sup>+</sup>
1.9356	C <sub>16</sub> Cl <sub>3</sub> H <sub>15</sub>	2.0647	C <sub>10</sub> H <sub>15</sub> <sup>+</sup> N•HBr
1.9359	Ba(C <sub>6</sub> H <sub>5</sub> )P <sup>+</sup> <sub>4</sub> •1.5H <sub>2</sub> O	2.0653	Hg(C <sub>5</sub> H <sub>5</sub> N) <sub>2</sub> Cl <sub>2</sub>
1.9378	C <sub>10</sub> H <sub>15</sub> <sup>+</sup> N•HI	2.0668	CH <sub>2</sub> :N <sup>+</sup> Se <sub>3</sub> K
1.9397	C <sup>+</sup> OHCH(NHC <sup>+</sup> CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> SCH <sub>3</sub>	2.0710	(C <sub>2</sub> H <sub>5</sub> )(C <sub>6</sub> H <sub>5</sub> )C <sub>5</sub> H <sub>3</sub> N <sup>+</sup>
1.9405	C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub>	2.0761	Co(C <sub>5</sub> H <sub>7</sub> <sup>+</sup> ) <sub>2</sub> •2H <sub>2</sub> O
1.9422	K <sub>3</sub> Co(CN) <sub>6</sub>	2.0788	C <sub>6</sub> H <sub>6</sub> •C <sub>6</sub> (N <sup>+</sup> ) <sub>2</sub> <sup>+</sup>
1.9438	C <sub>6</sub> H <sub>10</sub> <sup>+</sup>	2.0799	HgCl <sub>2</sub> •C <sub>9</sub> H <sub>6</sub> <sup>+</sup>
1.9439	C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> <sup>+</sup> Pd	2.0828	Fe(C <sub>27</sub> H <sub>24</sub> N <sub>4</sub> S <sub>2</sub> )(FeCl <sub>4</sub> ) <sub>2</sub> •C <sub>3</sub> H <sub>6</sub> O
1.9453	Co(C <sub>9</sub> H <sub>11</sub> ) <sub>2</sub> [P(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ] <sub>2</sub>	2.0888	[Co(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> Cl <sub>2</sub> ] <sub>2</sub> Cl•H <sub>2</sub> O
1.9483	(CH <sub>3</sub> )(C <sub>6</sub> H <sub>5</sub> )(C <sub>2</sub> H <sub>5</sub> C <sup>+</sup> )C <sub>5</sub> H <sub>8</sub> N <sup>+</sup> HCl	2.0911	C <sub>20</sub> H <sub>20</sub> <sup>+</sup>
1.9510	CH <sub>3</sub> C <sub>10</sub> H <sub>6</sub> CH <sub>3</sub>	2.0955	Cu(NH <sub>2</sub> CH <sub>2</sub> C <sup>+</sup> NCH <sub>2</sub> C <sup>+</sup> ) <sub>3</sub> •3H <sub>2</sub> O
1.9524	3C <sub>6</sub> H <sub>5</sub> C <sub>2</sub> C <sup>+</sup> CH <sub>3</sub> •Fe(C <sup>+</sup> ) <sub>3</sub>	2.0976	C <sub>10</sub> H <sub>15</sub> <sup>+</sup> N•HI
1.9533	C <sub>9</sub> H <sub>6</sub> NCl	2.0976	Ni(C <sub>5</sub> H <sub>7</sub> <sup>+</sup> ) <sub>2</sub> •2H <sub>2</sub> O
1.9542	C <sub>6</sub> H <sub>5</sub> •(CH:CH) <sub>3</sub> C <sub>6</sub> H <sub>5</sub>	2.1005	C <sub>7</sub> H <sub>7</sub> S <sup>+</sup> SN <sup>+</sup> •2H <sub>2</sub> O
1.9593	CH <sub>3</sub> H <sub>4</sub> C <sub>6</sub> •C <sub>6</sub> H <sub>2</sub> •CH <sub>3</sub> ClNH <sub>2</sub>	2.1017	CH <sub>3</sub> C•C•CH <sub>3</sub> •H <sub>2</sub> Fe <sub>2</sub> (C <sup>+</sup> ) <sub>8</sub>
1.9613	Cu(C <sub>15</sub> H <sub>11</sub> N <sub>3</sub> )Cl <sub>2</sub> •2H <sub>2</sub> O	2.1032	C <sub>6</sub> H <sub>3</sub> (N <sup>+</sup> ) <sub>2</sub> NH <sup>+</sup> N:CH•C <sub>6</sub> H <sub>5</sub>

P2<sub>1</sub>/c C<sub>2h</sub><sup>5</sup> No. 14 (continued)

## Organic (continued)

2.1055	(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>3</sub> Al	2.3198	Cu <sub>2</sub> Cl <sub>4</sub> (CH <sub>3</sub> CN) <sub>2</sub>
2.1061	HgBr <sub>2</sub> •C <sub>9</sub> H <sub>6</sub> O <sub>2</sub>	2.3205	C <sub>30</sub> H <sub>20</sub>
2.1135	Cs <sub>2</sub> (C <sub>12</sub> H <sub>4</sub> N <sub>4</sub> ) <sub>3</sub>	2.3218	(C <sub>6</sub> H <sub>5</sub> NCO) <sub>2</sub>
2.1227	C <sub>5</sub> H <sub>15</sub> Br <sub>10</sub> Hg	2.3228	C <sub>16</sub> H <sub>11</sub> N <sub>3</sub> O <sub>6</sub>
2.1233	C <sub>6</sub> H <sub>5</sub> (C≡C) <sub>4</sub> C <sub>6</sub> H <sub>5</sub>	2.3237	(C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> Se <sub>2</sub>
2.1253	C <sub>14</sub> H <sub>12</sub> O	2.3298	Cu(NCO) <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> NCO) <sub>2</sub>
2.1254	C <sub>6</sub> H <sub>5</sub> SC <sub>6</sub> H <sub>3</sub> CH <sub>3</sub> NCO <sub>2</sub>	2.3323	(ClC <sub>6</sub> H <sub>4</sub> Te) <sub>2</sub>
2.1303	(CH <sub>3</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>2</sub> •CF•CF•C <sub>6</sub> H <sub>5</sub>	2.3381	C <sub>6</sub> H <sub>7</sub> NOI <sub>2</sub>
2.1303	C <sub>10</sub> H <sub>5</sub> N <sub>3</sub> O <sub>6</sub>	2.3399	Cu(C <sub>6</sub> H <sub>6</sub> ON) <sub>2</sub> •2H <sub>2</sub> O
2.1315	C <sub>14</sub> H <sub>29</sub> Se <sub>3</sub> Na•0.5H <sub>2</sub> O	2.3413	C <sub>6</sub> H <sub>5</sub> •(C <sub>2</sub> N <sub>2</sub> O <sub>2</sub> )•C <sub>6</sub> H <sub>5</sub>
2.1363	Ga(C <sub>6</sub> H <sub>2</sub> COC <sub>6</sub> H <sub>2</sub> COC <sub>6</sub> H <sub>3</sub> ) <sub>3</sub>	2.3446	C <sub>18</sub> H <sub>19</sub> N <sub>2</sub> Br•HBr
2.1390	C <sub>10</sub> H <sub>9</sub> NCO <sub>3</sub> S•H <sub>2</sub> O	2.3464	CCl <sub>3</sub> CH(C <sub>6</sub> H <sub>4</sub> OC <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>
2.1395	C <sub>6</sub> H <sub>10</sub> ClBr	2.3489	Cu(C <sub>3</sub> H <sub>6</sub> NCO <sub>2</sub> ) <sub>2</sub> •6H <sub>2</sub> O
2.1439	C <sub>6</sub> H <sub>10</sub> Br <sub>2</sub>	2.3529	C <sub>15</sub> H <sub>13</sub> NCO <sub>2</sub> S
2.1507	C <sub>6</sub> Cl <sub>4</sub> (OH) <sub>2</sub>	2.3571	Cu(OH) <sub>2</sub> H <sub>2</sub> (C <sub>10</sub> H <sub>11</sub> N <sub>2</sub> O <sub>8</sub> )
2.1511	C <sub>6</sub> H <sub>10</sub> Cl <sub>2</sub>	2.3575	C <sub>6</sub> H <sub>3</sub> (NO <sub>2</sub> ) <sub>3</sub> •C <sub>6</sub> H <sub>7</sub> N
2.1511	[CH <sub>3</sub> O <sub>2</sub> C <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub> O	2.3627	C <sub>36</sub> H <sub>24</sub> Hg <sub>6</sub>
2.1646	C <sub>6</sub> Cl <sub>4</sub> (OH) <sub>2</sub>	2.3648	C <sub>16</sub> H <sub>33</sub> Se <sub>3</sub> Na•0.5H <sub>2</sub> O
2.1691	Cr(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>3</sub>	2.3671	C <sub>11</sub> H <sub>17</sub> NO•HBr
2.1699	Mn(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>3</sub>	2.3686	HCOOC(CH <sub>2</sub> ) <sub>9</sub> COOH
2.1719	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> C <sub>8</sub> H <sub>8</sub>	2.3724	C <sub>12</sub> H <sub>8</sub> S <sub>2</sub>
2.1755	C <sub>28</sub> H <sub>24</sub>	2.3726	UO <sub>2</sub> (C <sub>10</sub> H <sub>8</sub> NO) <sub>2</sub> •C <sub>10</sub> H <sub>8</sub> NO•H•CHCl <sub>3</sub>
2.1775	(CH <sub>3</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CF•CFC <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>	2.3818	C <sub>28</sub> H <sub>24</sub>
2.1817	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> P•C•C•P(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	2.3878	C <sub>4</sub> H <sub>8</sub> S <sub>2</sub> •2I <sub>2</sub>
2.1824	C <sub>16</sub> H <sub>8</sub> O <sub>2</sub> Se <sub>2</sub>	2.3887	C <sub>4</sub> H <sub>8</sub> SeSe•2I <sub>2</sub>
2.1835	C <sub>8</sub> H <sub>6</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>5</sub>	2.3916	C <sub>12</sub> H <sub>24</sub> Cl <sub>2</sub> N <sub>8</sub> S <sub>4</sub> Te•2H <sub>2</sub> O
2.1853	C <sub>6</sub> H <sub>10</sub> I <sub>2</sub>	2.3922	HCOOC(CH <sub>2</sub> ) <sub>3</sub> C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> (CH <sub>2</sub> ) <sub>3</sub> COOH
2.1860	C <sub>9</sub> H <sub>6</sub> NNaO <sub>2</sub> S	2.3971	K <sub>2</sub> V <sub>6</sub> (NCS) <sub>4</sub> •5H <sub>2</sub> O
2.1886	(C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ) <sub>3</sub> Rh	2.3988	C <sub>18</sub> H <sub>18</sub> N <sub>6</sub>
2.1917	[C <sub>2</sub> H <sub>5</sub> (NH <sub>2</sub> )CHCOO] <sub>2</sub> Cu	2.3991	Ni(OH) <sub>2</sub> H <sub>2</sub> [C <sub>10</sub> H <sub>11</sub> N <sub>2</sub> O <sub>8</sub> ]
2.1940	HCOOC(CH <sub>2</sub> ) <sub>8</sub> COOH	2.4017	CuC <sub>10</sub> H <sub>10</sub> O <sub>4</sub>
2.1965	Co(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>3</sub>	2.4040	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> CH) <sub>5</sub> C <sub>6</sub> H <sub>5</sub>
2.1997	C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> S	2.4056	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O
2.2004	C <sub>12</sub> H <sub>19</sub> ClN <sub>4</sub> O <sub>7</sub> P <sub>2</sub> •2H <sub>2</sub> O	2.4103	C <sub>10</sub> H <sub>8</sub> •C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>6</sub>
2.2032	(CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N) <sub>2</sub>	2.4152	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>
2.2105	C <sub>6</sub> H <sub>5</sub> •C(CH <sub>3</sub> ):CH•COOH	2.4182	C <sub>6</sub> H <sub>4</sub> BrCl
2.2122	C <sub>20</sub> H <sub>12</sub> •C <sub>6</sub> F <sub>6</sub>	2.4194	(NH <sub>4</sub> ) <sub>2</sub> V <sub>6</sub> (NCS) <sub>4</sub> •5H <sub>2</sub> O
2.2150	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> Cl(BF <sub>4</sub> )	2.4212	C <sub>23</sub> H <sub>16</sub> ON <sub>2</sub>
2.2154	C <sub>6</sub> H <sub>4</sub> ClI <sub>2</sub> O	2.4223	C <sub>11</sub> H <sub>17</sub> ON•HCl
2.2164	C <sub>14</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> Cu	2.4253	C <sub>6</sub> H <sub>5</sub> •C <sub>6</sub> H <sub>4</sub> •C <sub>6</sub> H <sub>5</sub>
2.2175	Ni(OH) <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CHNH) <sub>2</sub>	2.4280	Zn(C <sub>9</sub> H <sub>6</sub> ON) <sub>2</sub> •2H <sub>2</sub> O
2.2187	C <sub>21</sub> H <sub>16</sub>	2.4288	C <sub>6</sub> H <sub>5</sub> -C≡C-C≡C-C <sub>6</sub> H <sub>5</sub>
2.2205	Cu(C <sub>7</sub> H <sub>6</sub> NO) <sub>2</sub>	2.4313	C <sub>5</sub> H <sub>5</sub> Fe(CO) <sub>2</sub> Mn(CO) <sub>5</sub>
2.2222	Al(CH <sub>2</sub> COCH <sub>2</sub> COCH <sub>3</sub> ) <sub>3</sub>	2.4353	C <sub>14</sub> H <sub>11</sub> N
2.2230	Ni(C <sub>7</sub> H <sub>6</sub> NO) <sub>2</sub>	2.4357	C <sub>12</sub> H <sub>24</sub> Br <sub>2</sub> N <sub>8</sub> S <sub>4</sub> Te•2H <sub>2</sub> O
2.2263	MgCO <sub>3</sub> •3H <sub>2</sub> O	2.4358	CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> SeO <sub>2</sub> H
2.2390	C <sub>36</sub> H <sub>22</sub> N <sub>4</sub>	2.4416	ClC <sub>6</sub> H <sub>4</sub> SeO <sub>2</sub> H
2.2454	(ClC <sub>6</sub> H <sub>4</sub> Se) <sub>2</sub>	2.4545	C <sub>14</sub> H <sub>12</sub> N <sub>2</sub>
2.2460	C <sub>5</sub> H <sub>5</sub> NO <sub>2</sub>	2.4548	[(CH <sub>3</sub> ) <sub>4</sub> Si <sub>2</sub> O] <sub>2</sub>
2.2491	C <sub>14</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> Pd	2.4565	CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N:NC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub>
2.2495	C <sub>6</sub> H <sub>10</sub> Br <sub>2</sub>	2.4572	C <sub>6</sub> H <sub>5</sub> SeO <sub>2</sub> H
2.2547	C <sub>8</sub> H <sub>15</sub> NO <sub>2</sub> •HCl	2.4623	AlCl <sub>3</sub> •C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>
2.2550	C <sub>6</sub> H <sub>5</sub> •CF <sub>2</sub> •CF <sub>2</sub> •C <sub>6</sub> H <sub>5</sub>	2.4630	NO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> SeO <sub>2</sub> H
2.2615	C <sub>5</sub> H <sub>5</sub> NS	2.4689	C <sub>4</sub> H <sub>8</sub> Se <sub>2</sub> •2I <sub>2</sub>
2.2619	C <sub>10</sub> H <sub>18</sub> Br <sub>2</sub>	2.4697	(C <sub>6</sub> H <sub>5</sub> -CH <sub>2</sub> ) <sub>3</sub> N
2.2634	C <sub>10</sub> H <sub>5</sub> IN <sub>4</sub> O <sub>2</sub> S	2.4718	C <sub>8</sub> H <sub>7</sub> NS <sub>2</sub>
2.2659	C <sub>6</sub> H <sub>10</sub> (CO <sub>2</sub> CH <sub>3</sub> ) <sub>2</sub>	2.4740	CH <sub>3</sub> COOC <sub>6</sub> H <sub>4</sub> •C <sub>6</sub> H <sub>4</sub> F
2.2703	C <sub>16</sub> H <sub>16</sub> •AgNO <sub>3</sub>	2.4777	NaBr•2(CH <sub>3</sub> CO <sub>2</sub> NH <sub>2</sub> )
2.2713	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O	2.4784	C <sub>6</sub> H <sub>4</sub> (SH)COOH
2.2791	C <sub>13</sub> H <sub>6</sub> N	2.4805	(CH <sub>2</sub> OH) <sub>2</sub>
2.2805	C <sub>6</sub> H <sub>8</sub> O <sub>7</sub>	2.4852	(C <sub>20</sub> H <sub>16</sub> N <sub>4</sub> •HAsF <sub>4</sub> O) <sub>2</sub> •2CH <sub>3</sub> CN
2.2809	CH <sub>3</sub> COOC <sub>6</sub> H <sub>4</sub> •CH(C <sub>2</sub> H <sub>5</sub> )•CH(C <sub>2</sub> H <sub>5</sub> )•C <sub>6</sub> H <sub>4</sub> COOCH <sub>3</sub>	2.4870	C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub>
2.2857	Te(C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> S) <sub>2</sub> (S <sub>2</sub> O <sub>2</sub> CH <sub>3</sub> ) <sub>2</sub>	2.4950	C <sub>4</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> •H <sub>2</sub> O
2.2859	C <sub>35</sub> H <sub>21</sub> N <sub>5</sub>	2.4952	C <sub>6</sub> H <sub>4</sub> (CO) <sub>2</sub> NC <sub>6</sub> H <sub>2</sub>
2.2870	C <sub>20</sub> H <sub>12</sub> •C <sub>6</sub> F <sub>4</sub> O <sub>2</sub>	2.4970	C <sub>14</sub> H <sub>12</sub>
2.2899	C <sub>6</sub> H <sub>5</sub> Cl <sub>2</sub> I	2.4973	NH <sub>2</sub> CO(CH <sub>2</sub> ) <sub>4</sub> CH <sub>3</sub>
2.2932	C <sub>10</sub> H <sub>9</sub> BrN <sub>4</sub> O <sub>2</sub> S	2.5000	C <sub>6</sub> H <sub>4</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
2.2993	(OC <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> OH) <sub>2</sub> Cu	2.5018	Cu(C <sub>9</sub> H <sub>10</sub> NO) <sub>2</sub>
2.3009	[(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> Cl][BF <sub>4</sub> ]	2.5052	C <sub>6</sub> H <sub>3</sub> (NO <sub>2</sub> ) <sub>3</sub> •CH <sub>3</sub> •C <sub>6</sub> H <sub>6</sub> N
2.3019	C <sub>9</sub> H <sub>20</sub> BrN	2.5068	C <sub>10</sub> Cl <sub>8</sub>
2.3026	Hg(C <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> ) <sub>2</sub>	2.5204	C <sub>8</sub> H <sub>3</sub> O <sub>9</sub> Rb
2.3042	HCOOC <sub>6</sub> H <sub>4</sub> CO <sub>2</sub> NH <sub>2</sub>	2.5208	C <sub>4</sub> H <sub>9</sub> C <sub>2</sub> N
2.3054	C <sub>18</sub> H <sub>19</sub> N <sub>2</sub> Cl•HBr	2.5252	C <sub>12</sub> H <sub>8</sub> N <sub>2</sub>
2.3140	C <sub>26</sub> H <sub>16</sub>	2.5303	C <sub>6</sub> H <sub>5</sub> •N=N•C <sub>6</sub> H <sub>4</sub> •NH <sub>2</sub>

P<sub>2</sub>/c C<sub>2</sub><sup>5</sup><sub>2h</sub> No. 14 (continued)

## Organic (continued)

2.5335	[Pt(NH <sub>3</sub> ) <sub>4</sub> (CH <sub>3</sub> CN) <sub>2</sub> ]Cl <sub>2</sub> •H <sub>2</sub> O	2.8849	C <sub>6</sub> H <sub>5</sub> (C≡C) <sub>3</sub> C <sub>6</sub> H <sub>5</sub>
2.5336	C <sub>8</sub> H <sub>15</sub> Br	2.8919	C <sub>8</sub> H <sub>8</sub> S <sub>2</sub>
2.5355	C <sub>5</sub> H <sub>5</sub> FeB <sub>2</sub> C <sub>2</sub> H <sub>11</sub>	2.8980	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub>
2.5385	C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub>	2.9057	CH <sub>3</sub> •CH•(NH <sub>2</sub> )C <sub>6</sub> H <sub>4</sub> •NH•CH <sub>2</sub> •C <sub>6</sub> H <sub>5</sub>
2.5402	C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> O	2.9065	Br <sub>2</sub> C:CB <sub>2</sub> :C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>
2.5453	C <sub>40</sub> H <sub>56</sub>	2.9071	[H <sub>3</sub> C•C <sub>6</sub> H <sub>4</sub> •CH <sub>2</sub> •CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub> H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> •H <sub>2</sub> O
2.5500	C <sub>10</sub> H <sub>7</sub> NH <sub>2</sub>	2.9074	Br•C <sub>6</sub> H <sub>4</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>
2.5557	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> •HBr•H <sub>2</sub> O	2.9254	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> Si(OH) <sub>2</sub>
2.5609	C <sub>7</sub> H <sub>5</sub> NS <sub>2</sub>	2.9357	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> P <sub>2</sub> O <sub>4</sub>
2.5711	Zn(C <sub>5</sub> H <sub>4</sub> N•C <sub>5</sub> H <sub>3</sub> N•C <sub>5</sub> H <sub>4</sub> N)(NO <sub>3</sub> ) <sub>2</sub> •3H <sub>2</sub> O	2.9535	(CH <sub>2</sub> CHCH <sub>2</sub> ) <sub>2</sub> Si(OH) <sub>2</sub>
2.5735	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •C•(C <sub>6</sub> H <sub>2</sub> Br <sub>2</sub> O)	2.9547	H <sub>3</sub> C•C <sub>6</sub> H <sub>4</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>
2.5737	NO <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>	2.9551	C <sub>6</sub> (OH) <sub>4</sub> O <sub>2</sub> •2H <sub>2</sub> O
2.5807	C <sub>14</sub> H <sub>15</sub> N	2.9554	C <sub>20</sub> H <sub>12</sub> N <sub>2</sub>
2.5813	C <sub>15</sub> H <sub>24</sub> •2AgNO <sub>3</sub>	2.9642	C <sub>14</sub> H <sub>8</sub> O <sub>4</sub>
2.5866	C <sub>18</sub> H <sub>37</sub> S <sub>3</sub> Na•0.5H <sub>2</sub> O	2.9652	C <sub>10</sub> H <sub>4</sub> NOBr <sub>5</sub>
2.5878	C <sub>12</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>6</sub>	2.9682	C <sub>14</sub> H <sub>8</sub> O <sub>4</sub>
2.5985	(CH <sub>3</sub> ) <sub>2</sub> C(OCH <sub>3</sub> )C(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> HgSCN	2.9825	C <sub>8</sub> H <sub>5</sub> NO <sub>2</sub>
2.6020	H <sub>2</sub> N(CH <sub>2</sub> ) <sub>5</sub> C <sub>6</sub> H <sub>5</sub>	2.9899	C <sub>4</sub> N <sub>2</sub> Br(NH <sub>2</sub> ) <sub>2</sub> O
2.6027	C <sub>10</sub> H <sub>7</sub> OH	3.0056	C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> S
2.6027	C <sub>15</sub> H <sub>15</sub> N•(NO <sub>2</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>2</sub> Cl	3.0065	C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> O
2.6096	KBCl <sub>3</sub>	3.0102	C <sub>22</sub> H <sub>24</sub> O <sub>6</sub>
2.6199	Cu <sub>3</sub> Cl <sub>6</sub> (CH <sub>3</sub> CN) <sub>2</sub>	3.0185	C <sub>10</sub> H <sub>7</sub> Cl
2.6377	C <sub>38</sub> H <sub>18</sub>	3.0225	C <sub>17</sub> H <sub>14</sub>
2.6435	Mg(C <sub>4</sub> H <sub>2</sub> N <sub>3</sub> O <sub>4</sub> ) <sub>2</sub>	3.0245	Mg(H <sub>2</sub> O) <sub>6</sub> [MgC <sub>6</sub> H <sub>5</sub> O <sub>7</sub> (H <sub>2</sub> O)] <sub>2</sub> •2H <sub>2</sub> O
2.6440	C <sub>6</sub> H <sub>5</sub> N <sub>2</sub> C <sub>6</sub> H <sub>5</sub>	3.0263	C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub>
2.6548	C <sub>22</sub> H <sub>20</sub> O <sub>4</sub>	3.0267	C <sub>19</sub> H <sub>19</sub> N
2.6573	Br•(OH)•C <sub>6</sub> H <sub>3</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>	3.0298	Cu <sub>5</sub> Cl <sub>10</sub> (C <sub>3</sub> H <sub>7</sub> OH) <sub>2</sub>
2.6613	H <sub>3</sub> CC(CH <sub>2</sub> ) <sub>10</sub> CO <sub>2</sub> H	3.0395	C <sub>17</sub> H <sub>14</sub>
2.6722	C <sub>21</sub> H <sub>15</sub> Cl <sub>4</sub> S <sub>2</sub>	3.0455	NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> SCN
2.6731	C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	3.0464	Cu(CH <sub>3</sub> COCH <sub>2</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>
2.6793	C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>2</sub>	3.0494	C <sub>18</sub> H <sub>18</sub>
2.6928	(C <sub>6</sub> H <sub>5</sub> C) <sub>2</sub>	3.0524	ReOCl <sub>3</sub> [P(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ]
2.7054	C <sub>6</sub> H <sub>5</sub> CHCH <sub>2</sub> •PdCl <sub>2</sub>	3.0538	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>
2.7062	NH <sub>2</sub> CO(CH <sub>2</sub> ) <sub>5</sub> CH <sub>3</sub>	3.0562	NH <sub>2</sub> CO(CH <sub>2</sub> ) <sub>6</sub> CH <sub>3</sub>
2.7111	(PC <sub>6</sub> H <sub>5</sub> ) <sub>5</sub>	3.0672	C <sub>10</sub> H <sub>7</sub> •CH <sub>3</sub>
2.7201	C <sub>14</sub> H <sub>10</sub> O <sub>2</sub>	3.0767	C <sub>16</sub> H <sub>16</sub> Fe(CO) <sub>3</sub>
2.7225	Cu(SCN) <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub> •Cu(SCN)(NH <sub>3</sub> )	3.0787	C <sub>16</sub> H <sub>10</sub> N <sub>2</sub>
2.7273	C <sub>7</sub> H <sub>11</sub> NO <sub>3</sub>	3.0816	C <sub>30</sub> H <sub>18</sub>
2.7325	CH <sub>3</sub> CO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> •C <sub>6</sub> H <sub>4</sub> CO <sub>2</sub> H	3.0851	Te(S <sub>2</sub> CH <sub>3</sub> ) <sub>2</sub>
2.7348	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> P:ClCOCH <sub>3</sub> •ClCOCH <sub>3</sub> :NC <sub>6</sub> H <sub>4</sub> Br	3.0937	(NH <sub>2</sub> (CH <sub>2</sub> ) <sub>4</sub> ) <sub>2</sub> (CH <sub>2</sub> CH <sub>2</sub> CO <sub>2</sub> H) <sub>2</sub>
2.7368	C <sub>6</sub> H <sub>7</sub> N <sub>3</sub> O <sub>3</sub>	3.0979	S(S <sub>2</sub> CH <sub>3</sub> ) <sub>2</sub>
2.7397	Cl•C <sub>6</sub> H(CH <sub>3</sub> ) <sub>4</sub>	3.1033	Se(S <sub>2</sub> CH <sub>3</sub> ) <sub>2</sub>
2.7403	LiC <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> H	3.1050	Cu(O <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CO <sub>2</sub> ) <sub>2</sub>
2.7435	(C <sub>6</sub> H <sub>5</sub> •CH:CH <sub>2</sub> •PdCl <sub>2</sub> ) <sub>2</sub>	3.1135	Fe(C <sub>5</sub> H <sub>4</sub> CH <sub>2</sub> CH <sub>2</sub> CO <sub>2</sub> C <sub>5</sub> H <sub>4</sub> )
2.7441	C <sub>13</sub> H <sub>10</sub> N <sub>4</sub> O <sub>6</sub>	3.1148	C <sub>6</sub> H <sub>5</sub> •CH:CH•CO <sub>2</sub> NH <sub>2</sub>
2.7491	C <sub>13</sub> H <sub>13</sub> N <sub>2</sub> O	3.1179	C <sub>12</sub> H <sub>7</sub> N <sub>4</sub> O <sub>6</sub> I
2.7518	C <sub>14</sub> H <sub>10</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	3.1214	LiI•(CH <sub>3</sub> ) <sub>2</sub> NCH <sub>3</sub>
2.7526	C <sub>14</sub> H <sub>12</sub>	3.1242	[C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>3</sub> ] <sub>2</sub> [CuCl <sub>4</sub> ]
2.7566	C <sub>14</sub> H <sub>8</sub> O <sub>4</sub>	3.1489	C <sub>14</sub> H <sub>10</sub>
2.7615	C <sub>10</sub> H <sub>7</sub> OH	3.2023	C <sub>4</sub> H <sub>3</sub> N <sub>3</sub> O <sub>5</sub> •3H <sub>2</sub> O
2.7626	C <sub>20</sub> H <sub>12</sub> •C <sub>6</sub> (N <sub>2</sub> O <sub>2</sub> ) <sub>3</sub>	3.2067	Zn(C <sub>3</sub> H <sub>5</sub> SO <sub>2</sub> ) <sub>2</sub>
2.7707	BrC <sub>6</sub> H(CH <sub>3</sub> ) <sub>4</sub>	3.2089	(C <sub>9</sub> H <sub>10</sub> NO) <sub>2</sub> Pd
2.7728	(C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> )FeCl	3.2090	C <sub>24</sub> H <sub>18</sub>
2.7873	Pd(C <sub>7</sub> H <sub>5</sub> O <sub>2</sub> N) <sub>2</sub>	3.2106	ClC <sub>6</sub> H <sub>4</sub> CH:CHCO <sub>2</sub> CH <sub>3</sub>
2.7905	H <sub>3</sub> CC(CH <sub>2</sub> ) <sub>11</sub> CO <sub>2</sub> H	3.2129	C <sub>6</sub> H <sub>5</sub> (C≡C) <sub>5</sub> C <sub>6</sub> H <sub>5</sub>
2.8083	C <sub>17</sub> H <sub>14</sub>	3.2136	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub>
2.8103	Fe(C <sub>5</sub> H <sub>4</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	3.2143	Pb[SC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>4</sub> Cl <sub>2</sub>
2.8109	C <sub>6</sub> H <sub>5</sub> NH <sub>3</sub> Br	3.2235	C <sub>16</sub> H <sub>10</sub>
2.8155	(C <sub>9</sub> H <sub>6</sub> NO) <sub>2</sub> Pd	3.2320	C <sub>18</sub> H <sub>14</sub>
2.8166	C <sub>5</sub> H <sub>5</sub> N•BF <sub>3</sub>	3.2487	C <sub>12</sub> H <sub>10</sub> O <sub>2</sub>
2.8205	C <sub>6</sub> H <sub>2</sub> (NO <sub>2</sub> ) <sub>3</sub> NHC <sub>6</sub> H <sub>5</sub>	3.2587	C <sub>6</sub> H <sub>5</sub> •CH•OH•CO <sub>2</sub> C <sub>6</sub> H <sub>5</sub>
2.8225	C <sub>20</sub> H <sub>18</sub> Cl <sub>2</sub>	3.2732	H <sub>3</sub> C•C <sub>6</sub> H <sub>4</sub> •CH:CH•CO <sub>2</sub> H
2.8310	Ni(C <sub>8</sub> H <sub>4</sub> N <sub>3</sub> S) <sub>2</sub>	3.2910	C <sub>6</sub> H <sub>2</sub> N <sub>4</sub> O <sub>4</sub> Rb <sub>2</sub> •2H <sub>2</sub> O
2.8340	Ni(O <sub>2</sub> C <sub>6</sub> H <sub>4</sub> •CH:NH <sub>2</sub> ) <sub>2</sub>	3.2997	C <sub>5</sub> H <sub>11</sub> CO <sub>2</sub> K
2.8393	C <sub>7</sub> H <sub>9</sub> NO	3.3000	C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> •2H <sub>2</sub> O
2.8557	C <sub>10</sub> H <sub>4</sub> (NO <sub>2</sub> ) <sub>4</sub>	3.3030	(C <sub>2</sub> H <sub>5</sub> O) <sub>2</sub> P <sub>2</sub> OSK
2.8594	C <sub>27</sub> H <sub>16</sub> O <sub>2</sub>	3.3138	C <sub>18</sub> H <sub>16</sub> (OH) <sub>2</sub>
2.8600	Cl•C <sub>6</sub> H <sub>4</sub> •CH:CH•CO <sub>2</sub> H	3.3163	C <sub>11</sub> H <sub>10</sub> O <sub>2</sub>
2.8627	C <sub>4</sub> H <sub>2</sub> O <sub>4</sub> •2H <sub>2</sub> O	3.3200	C <sub>18</sub> H <sub>10</sub>
2.8715	C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>3</sub>	3.3206	ClC <sub>6</sub> H <sub>4</sub> (C <sub>2</sub> H <sub>5</sub> )C•C(C <sub>2</sub> H <sub>5</sub> )C <sub>6</sub> H <sub>4</sub> Cl
2.8745	CH <sub>3</sub> CO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> •CH <sub>2</sub> CO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> •CO <sub>2</sub> CH <sub>3</sub>	3.3282	(Br•C <sub>6</sub> H <sub>4</sub> NO) <sub>2</sub>
2.8817	C <sub>20</sub> H <sub>19</sub> BrN <sub>2</sub> O	3.3337	C <sub>24</sub> H <sub>12</sub>
2.8825	C <sub>6</sub> (CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> ) <sub>3</sub>	3.3423	C <sub>14</sub> H <sub>8</sub> O <sub>2</sub>
2.8842	C <sub>6</sub> Br <sub>4</sub> O <sub>2</sub>	3.3432	S <sub>2</sub> (Se <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>

P2<sub>1</sub>/c C<sub>2h</sub><sup>5</sup> No. 14 (continued)

## Organic (continued)

3.3544	C <sub>7</sub> H <sub>4</sub> Cl <sub>4</sub> NCl	3.7696	C <sub>7</sub> H <sub>5</sub> Cl <sub>2</sub> Na
3.3670	C <sub>5</sub> H <sub>5</sub> N <sub>3</sub> θ	3.7723	(CH <sub>3</sub> ) <sub>2</sub> •C <sub>6</sub> H <sub>3</sub> •Cθ•θH
3.3681	C <sub>6</sub> H <sub>4</sub> (CθθK) <sub>2</sub>	3.7759	C <sub>6</sub> H <sub>5</sub> CH:CHCθθCH <sub>3</sub>
3.3883	C <sub>10</sub> H <sub>9</sub> Nθ <sub>2</sub>	3.7850	C <sub>6</sub> I <sub>6</sub>
3.3935	(CH <sub>3</sub> ) <sub>4</sub> Si <sub>2</sub> θ(θH) <sub>2</sub>	3.7873	Br(Nθ <sub>2</sub> )C <sub>6</sub> H <sub>3</sub> •CHθ
3.4000	C <sub>17</sub> H <sub>16</sub> θ	3.7946	C <sub>16</sub> H <sub>8</sub> θ <sub>4</sub>
3.4034	Cl <sub>2</sub> C <sub>6</sub> H <sub>3</sub> NH <sub>2</sub>	3.8023	C <sub>16</sub> H <sub>16</sub> θ <sub>4</sub>
3.4073	(CCl <sub>3</sub> ) <sub>2</sub> S <sub>3</sub>	3.8182	C <sub>10</sub> H <sub>16</sub> NH <sub>2</sub> •HCl
3.4179	(CCl <sub>3</sub> CHθ) <sub>3</sub>	3.8189	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>8</sub> CθNH <sub>2</sub>
3.4268	C <sub>7</sub> H <sub>5</sub> Iθ <sub>3</sub>	3.8191	C <sub>10</sub> H <sub>12</sub> Cl <sub>2</sub>
3.4272	C <sub>40</sub> H <sub>58</sub>	3.8300	C <sub>6</sub> Br <sub>5</sub> Cl
3.4376	Te(S <sub>2</sub> CθC <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	3.8346	C <sub>6</sub> Cl <sub>6</sub>
3.4529	(C <sub>6</sub> H <sub>5</sub> Sθ <sub>4</sub> ) <sub>2</sub> (Ni•θH <sub>2</sub> θ)	3.8347	C <sub>32</sub> H <sub>16</sub> BeN <sub>8</sub>
3.4560	(CH <sub>3</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>2</sub> •CF:CF•C <sub>6</sub> H <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub>	3.8398	C <sub>6</sub> Cl <sub>5</sub> Br
3.4598	C <sub>14</sub> H <sub>14</sub>	3.8435	C <sub>6</sub> Br <sub>6</sub>
3.4609	C <sub>6</sub> H <sub>3</sub> Cl <sub>2</sub> NH <sub>2</sub>	3.8546	C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub>
3.4812	(Nθ <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> CθθC <sub>2</sub> H <sub>5</sub>	3.8552	C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> θ
3.4937	C <sub>6</sub> H <sub>13</sub> Nθ <sub>2</sub>	3.8620	C <sub>6</sub> Cl <sub>6</sub>
3.5116	C <sub>3</sub> H <sub>5</sub> BrN <sub>2</sub> S <sub>2</sub> •H <sub>2</sub> θ	3.8667	C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> ) <sub>2</sub>
3.5186	C <sub>42</sub> H <sub>18</sub>	3.8711	FC <sub>6</sub> Cl <sub>5</sub>
3.5263	C <sub>4</sub> N <sub>2</sub> Br(NH <sub>2</sub> ) <sub>2</sub> H	3.8763	C <sub>6</sub> (CH <sub>3</sub> ) <sub>2</sub> Br <sub>4</sub>
3.5330	(C <sub>9</sub> H <sub>6</sub> N) <sub>2</sub>	3.8763	C <sub>6</sub> (CH <sub>3</sub> ) <sub>2</sub> Br <sub>4</sub>
3.5344	θNC <sub>5</sub> H <sub>4</sub> CH <sub>2</sub> θH	3.8882	(CH <sub>2</sub> ) <sub>16</sub> (CθθH) <sub>2</sub>
3.5409	LiRbHCθ <sub>2</sub> CH <sub>2</sub> CθHCθ <sub>2</sub> CH <sub>2</sub> Cθ <sub>2</sub> •H <sub>2</sub> θ	3.8907	SC <sub>4</sub> H <sub>3</sub> •Cθ•θH
3.5412	BrC <sub>6</sub> H <sub>4</sub> NHNCC <sub>6</sub> H <sub>4</sub> Br	3.9046	C <sub>8</sub> H <sub>9</sub> Nθ <sub>2</sub>
3.5443	C <sub>25</sub> H <sub>22</sub>	3.9098	θC(C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> S
3.5450	C <sub>20</sub> H <sub>12</sub> N <sub>2</sub> θ <sub>2</sub>	3.9236	(C <sub>6</sub> H <sub>4</sub> Cl) <sub>2</sub> CHCCL <sub>3</sub>
3.5487	C <sub>13</sub> H <sub>8</sub> θ <sub>3</sub> N <sub>2</sub>	3.9284	NH <sub>2</sub> Cθ(CH <sub>2</sub> ) <sub>5</sub> CH <sub>3</sub>
3.5489	BrC <sub>6</sub> H <sub>4</sub> CH:CHCθθCH <sub>3</sub>	3.9285	CH <sub>3</sub> S•C(:NH)NH <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> Cl•CθθH
3.5532	CH <sub>3</sub> SCH <sub>2</sub> •CH <sub>2</sub> •CH(NH <sub>2</sub> )CθθH	3.9376	C <sub>6</sub> H <sub>5</sub> Cθ•NH•CSe•NH•C <sub>6</sub> H <sub>5</sub>
3.5535	(C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> ) <sub>2</sub> Pθ <sub>4</sub> H	3.9520	C <sub>14</sub> H <sub>10</sub> θ
3.5539	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> θ <sub>4</sub> •H <sub>2</sub> θ	3.9548	C <sub>10</sub> H <sub>5</sub> Brθ <sub>2</sub>
3.5548	C <sub>8</sub> H <sub>10</sub> θ	3.9703	SeC <sub>4</sub> H <sub>3</sub> •Cθ•θH
3.5590	C <sub>14</sub> H <sub>6</sub> Br <sub>2</sub> θ <sub>2</sub>	3.9824	C <sub>14</sub> H <sub>8</sub> θ <sub>2</sub>
3.5601	Zn(C <sub>6</sub> H <sub>5</sub> Sθ <sub>3</sub> ) <sub>2</sub> •6H <sub>2</sub> θ	4.0052	C <sub>16</sub> H <sub>12</sub> CdN <sub>2</sub> θ <sub>2</sub>
3.5626	Nθ <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> •SθCH <sub>3</sub>	4.0067	Fe(C <sub>5</sub> H <sub>4</sub> CθθC <sub>3</sub> H <sub>5</sub> θ) <sub>2</sub>
3.5713	C <sub>14</sub> H <sub>16</sub> BrNθ <sub>3</sub>	4.0091	C <sub>30</sub> H <sub>22</sub>
3.5747	C <sub>25</sub> H <sub>24</sub>	4.0095	(CH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> •Sθ <sub>3</sub> ) <sub>2</sub> Zn•6H <sub>2</sub> θ
3.5759	Mg(C <sub>6</sub> H <sub>5</sub> Sθ <sub>3</sub> ) <sub>2</sub> •6H <sub>2</sub> θ	4.0096	(C <sub>2</sub> H <sub>5</sub> )(C <sub>5</sub> H <sub>4</sub> N)C <sub>5</sub> H <sub>5</sub> Nθ <sub>2</sub>
3.5765	Pd(C <sub>13</sub> H <sub>8</sub> Nθ <sub>2</sub> ) <sub>2</sub>	4.0097	C <sub>12</sub> H <sub>7</sub> N <sub>4</sub> θ <sub>6</sub> I
3.5779	(C <sub>6</sub> H <sub>5</sub> ) <sub>6</sub> P <sub>6</sub>	4.0107	C <sub>14</sub> H <sub>8</sub> θ <sub>2</sub>
3.5808	RbC <sub>9</sub> H <sub>14</sub> NSθ <sub>3</sub>	4.0184	C <sub>20</sub> H <sub>10</sub> θ <sub>4</sub>
3.5887	Li(NH <sub>4</sub> )HCθ <sub>2</sub> CH <sub>2</sub> CθHCθ <sub>2</sub> CH <sub>2</sub> Cθ <sub>2</sub> •H <sub>2</sub> θ	4.0256	(CH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> Sθ <sub>3</sub> ) <sub>2</sub> Mg•6H <sub>2</sub> θ
3.5931	C <sub>6</sub> H <sub>13</sub> Nθ <sub>2</sub>	4.0270	C <sub>6</sub> H <sub>9</sub> CLN <sub>2</sub> θ <sub>4</sub>
3.6197	ClC <sub>6</sub> H <sub>4</sub> •NHθN:NC <sub>6</sub> H <sub>4</sub> Cl	4.0451	Br(CH <sub>2</sub> ) <sub>10</sub> CθθH
3.6327	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>3</sub> CθθH	4.0508	C <sub>19</sub> H <sub>16</sub> Nθ <sub>3</sub>
3.6380	C <sub>6</sub> H <sub>5</sub> Nθ <sub>2</sub>	4.0509	C <sub>10</sub> H <sub>6</sub> BrNθ <sub>2</sub>
3.6514	C <sub>32</sub> N <sub>8</sub> H <sub>16</sub> Cu	4.0511	C <sub>7</sub> H <sub>15</sub> CθθK
3.6560	C <sub>6</sub> H <sub>5</sub> •C <sub>3</sub> HNθ•C <sub>6</sub> H <sub>4</sub> •C <sub>3</sub> HNθ•C <sub>6</sub> H <sub>5</sub>	4.0707	C <sub>5</sub> H <sub>6</sub> N <sub>3</sub> Cl
3.6590	C <sub>33</sub> H <sub>17</sub> N <sub>7</sub> Cu	4.0719	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> •BθH <sub>11</sub> :NHC <sub>2</sub> H <sub>5</sub>
3.6597	C <sub>6</sub> H <sub>5</sub> As	4.0871	C <sub>6</sub> H <sub>5</sub> C <sub>3</sub> H <sub>2</sub> S <sub>2</sub> I
3.6674	C <sub>33</sub> H <sub>19</sub> N <sub>7</sub>	4.0901	C <sub>19</sub> H <sub>14</sub>
3.6674	C <sub>32</sub> N <sub>8</sub> H <sub>18</sub>	4.1012	AgNθ <sub>3</sub> •S <sub>3</sub> C <sub>3</sub> H <sub>6</sub>
3.6743	C <sub>6</sub> H <sub>5</sub> As	4.1042	C <sub>12</sub> H <sub>8</sub> I <sub>2</sub>
3.6795	C <sub>7</sub> H <sub>6</sub> CLNθ <sub>2</sub>	4.1175	C <sub>12</sub> H <sub>8</sub> Br <sub>2</sub> N <sub>2</sub> θ
3.6865	C <sub>6</sub> H <sub>5</sub> As	4.1197	C <sub>10</sub> H <sub>5</sub> Br <sub>2</sub> N
3.6907	ClC <sub>6</sub> H <sub>4</sub> CF:CFC <sub>6</sub> H <sub>4</sub> Cl	4.1426	C <sub>32</sub> H <sub>14</sub>
3.6915	CH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> •N:N•NH•C <sub>6</sub> H <sub>4</sub> •CH <sub>3</sub>	4.1481	C <sub>24</sub> H <sub>16</sub>
3.6923	C <sub>6</sub> H <sub>5</sub> NH-N-N-C <sub>6</sub> H <sub>5</sub>	4.1488	CH <sub>3</sub> Cθ•Cθ•θNa
3.6988	CH <sub>2</sub> (C <sub>6</sub> H <sub>4</sub> Br) <sub>2</sub>	4.1509	[(HθCH <sub>2</sub> CH <sub>2</sub> N:CH)•C <sub>6</sub> H <sub>4</sub> θ] <sub>2</sub> Cu
3.7049	C <sub>32</sub> H <sub>16</sub> N <sub>8</sub> Ni	4.1513	(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> Ni <sub>2</sub> •HC•CC <sub>4</sub> H <sub>9</sub>
3.7068	FC <sub>6</sub> Br <sub>5</sub>	4.1553	C <sub>7</sub> H <sub>15</sub> CθθK
3.7172	NH <sub>2</sub> C <sub>10</sub> H <sub>5</sub> θ <sub>2</sub>	4.1556	C <sub>10</sub> H <sub>6</sub> (CHθNθ <sub>2</sub> ) <sub>2</sub>
3.7233	C <sub>32</sub> H <sub>16</sub> FθN <sub>8</sub>	4.1648	C <sub>6</sub> H <sub>4</sub> F•CθθH
3.7241	C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> θ <sub>3</sub>	4.1760	C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> Niθ <sub>2</sub>
3.7267	IC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> •C <sub>6</sub> H <sub>3</sub> (Nθ <sub>2</sub> ) <sub>3</sub>	4.1937	C <sub>12</sub> H <sub>4</sub> CL <sub>4</sub> N <sub>2</sub>
3.7389	C <sub>32</sub> H <sub>16</sub> MnN <sub>8</sub>	4.1990	BrC <sub>6</sub> H <sub>4</sub> NCC <sub>6</sub> H <sub>4</sub> Br
3.7400	C <sub>32</sub> H <sub>16</sub> CoN <sub>8</sub>	4.2104	FC <sub>6</sub> H <sub>4</sub> CθNH <sub>2</sub>
3.7424	C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> •2H <sub>2</sub> θ	4.2335	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> θS
3.7500	[C <sub>2</sub> H <sub>5</sub> CθNH(CH <sub>2</sub> ) <sub>3</sub> ] <sub>2</sub>	4.2581	(CH <sub>2</sub> ) <sub>6</sub> N <sub>4</sub> •C <sub>6</sub> H <sub>4</sub> (θH)(CθθH)
3.7506	C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> θ <sub>2</sub>	4.2607	C <sub>6</sub> H <sub>5</sub> •CθθH
3.7558	C <sub>9</sub> SθH <sub>7</sub>	4.2775	C <sub>4</sub> H <sub>3</sub> CL <sub>2</sub> N <sub>3</sub>
3.7580	C <sub>12</sub> H <sub>18</sub> CuN <sub>2</sub> θ <sub>2</sub> •H <sub>2</sub> θ	4.3183	C <sub>6</sub> H <sub>5</sub> (C C) <sub>4</sub> C <sub>6</sub> H <sub>5</sub>

P2<sub>1</sub>/c C<sub>2h</sub><sup>5</sup> No. 14 (continued)

## Organic (continued)

4.3424	C <sub>23</sub> H <sub>12</sub> N <sub>2</sub> Cl <sub>2</sub>	5.6992	RbC <sub>7</sub> H <sub>5</sub> Cl <sub>3</sub> •C <sub>7</sub> H <sub>6</sub> Cl <sub>3</sub> •H <sub>2</sub> O
4.3582	(CH <sub>2</sub> ) <sub>7</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	5.7090	C <sub>11</sub> H <sub>23</sub> C <sub>6</sub> H <sub>5</sub>
4.3629	N <sub>6</sub> •C <sub>6</sub> H <sub>4</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>	5.7143	Cl <sub>2</sub> •C <sub>6</sub> H <sub>3</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>
4.3772	C <sub>6</sub> H <sub>5</sub> C <sub>6</sub> NH <sub>2</sub>	5.7404	NH <sub>4</sub> C <sub>7</sub> H <sub>5</sub> Cl <sub>3</sub> •C <sub>7</sub> H <sub>6</sub> Cl <sub>3</sub> •H <sub>2</sub> O
4.3779	C <sub>3</sub> H <sub>7</sub> •C <sub>6</sub> H <sub>4</sub> CH:CH•C <sub>6</sub> H <sub>5</sub>	5.7422	C <sub>30</sub> H <sub>14</sub> Cl <sub>2</sub>
4.3791	C <sub>26</sub> H <sub>40</sub>	5.7732	KC <sub>7</sub> H <sub>5</sub> Cl <sub>3</sub> •C <sub>7</sub> H <sub>6</sub> Cl <sub>3</sub> •H <sub>2</sub> O
4.3878	CH <sub>3</sub> •Br•C <sub>6</sub> H <sub>3</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>	5.8007	BrC <sub>6</sub> H <sub>4</sub> •CH <sub>2</sub> •CH <sub>2</sub> •C <sub>6</sub> H <sub>5</sub>
4.4007	Cd(C <sub>4</sub> H <sub>9</sub> SCSS) <sub>2</sub>	5.8384	C <sub>20</sub> H <sub>41</sub> S <sub>4</sub> Na•0.25H <sub>2</sub> O
4.4389	C <sub>6</sub> Br <sub>6</sub> •C <sub>6</sub> H <sub>2</sub> Br <sub>4</sub>	5.8505	ClC <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub>
4.4417	NH <sub>2</sub> C <sub>6</sub> (CH <sub>2</sub> ) <sub>10</sub> CH <sub>3</sub>	5.8560	C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>
4.4539	AgCl•2NH <sub>2</sub> CSNH <sub>2</sub>	5.9098	C <sub>14</sub> H <sub>9</sub> N <sub>2</sub> O <sub>2</sub>
4.4573	CH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>	5.9231	C <sub>17</sub> H <sub>35</sub> C <sub>6</sub> H <sub>5</sub>
4.4767	NH <sub>4</sub> C(CN) <sub>3</sub>	5.9797	C <sub>6</sub> H <sub>5</sub> •C•C•I-HNC <sub>4</sub> H <sub>8</sub> O
4.4769	Cu(C <sub>10</sub> H <sub>6</sub> Cl <sub>2</sub> •N <sub>2</sub> •C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	6.0078	(NH <sub>2</sub> ClC <sub>6</sub> H <sub>3</sub> ) <sub>2</sub>
4.5116	K <sub>3</sub> Co(CN) <sub>6</sub>	6.0256	C <sub>21</sub> H <sub>12</sub> N <sub>4</sub>
4.5121	C <sub>20</sub> H <sub>20</sub> O	6.1180	C <sub>10</sub> H <sub>7</sub> C <sub>6</sub> H <sub>5</sub>
4.6017	CuC <sub>14</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>	6.1924	C <sub>15</sub> H <sub>31</sub> Cl <sub>2</sub> •C <sub>15</sub> H <sub>31</sub> Cl <sub>2</sub> Na
4.6096	C <sub>21</sub> H <sub>20</sub> Br <sub>2</sub> O <sub>8</sub>	6.2386	(CH <sub>2</sub> ) <sub>11</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
4.6333	NH <sub>2</sub> C <sub>6</sub> (CH <sub>2</sub> ) <sub>11</sub> CH <sub>3</sub>	6.2402	C <sub>22</sub> H <sub>12</sub> O <sub>6</sub>
4.6857	C <sub>36</sub> H <sub>26</sub>	6.2758	C <sub>14</sub> H <sub>7</sub> F <sub>6</sub> O <sub>2</sub>
4.7025	C <sub>18</sub> H <sub>16</sub> O	6.3835	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>12</sub> C <sub>6</sub> H <sub>5</sub>
4.7069	C <sub>14</sub> H <sub>9</sub> N <sub>2</sub> O <sub>2</sub>	6.4441	C <sub>20</sub> H <sub>38</sub> Cl <sub>4</sub>
4.7120	C <sub>14</sub> H <sub>6</sub> I <sub>2</sub> F <sub>2</sub>	6.4738	C <sub>7</sub> H <sub>7</sub> N <sub>3</sub>
4.7263	C <sub>6</sub> H <sub>4</sub> (C <sub>6</sub> H <sub>5</sub> •C <sub>2</sub> H <sub>4</sub> OH) <sub>2</sub>	6.4921	C <sub>13</sub> H <sub>27</sub> C <sub>6</sub> H <sub>5</sub>
4.7500	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>7</sub> C <sub>6</sub> H <sub>5</sub>	6.5076	FC <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub>
4.7977	C <sub>10</sub> H <sub>7</sub> NH•C <sub>6</sub> H <sub>3</sub> (Cl) <sub>2</sub> C <sub>6</sub> H <sub>5</sub>	6.5131	C <sub>7</sub> H <sub>7</sub> Cl <sub>3</sub> N
4.8152	(C <sub>6</sub> H <sub>4</sub> Br) <sub>2</sub> C <sub>6</sub> H <sub>5</sub>	6.5160	Cu(C <sub>9</sub> H <sub>6</sub> N <sub>6</sub> ) <sub>2</sub>
4.8258	C <sub>8</sub> H <sub>10</sub> O	6.5261	C <sub>24</sub> H <sub>50</sub>
4.8530	C <sub>32</sub> H <sub>16</sub> N <sub>8</sub> Pt	6.5849	C <sub>18</sub> H <sub>24</sub> O <sub>2</sub>
4.8673	C <sub>9</sub> H <sub>19</sub> C <sub>6</sub> H <sub>5</sub>	6.8699	C <sub>17</sub> H <sub>35</sub> Cl <sub>2</sub> •C <sub>17</sub> H <sub>35</sub> Cl <sub>2</sub> Na
4.9149	C <sub>6</sub> H <sub>5</sub> C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	6.9321	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> C <sub>4</sub> H <sub>4</sub>
4.9419	C <sub>9</sub> H <sub>19</sub> C <sub>6</sub> H <sub>5</sub>	7.0370	C <sub>5</sub> H <sub>5</sub> N•C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>7</sub>
4.9438	C <sub>14</sub> H <sub>6</sub> I <sub>2</sub> O <sub>2</sub>	7.1714	C <sub>11</sub> H <sub>9</sub> N <sub>2</sub> O•0.25H <sub>2</sub> O
4.9875	NH <sub>2</sub> C <sub>6</sub> (CH <sub>2</sub> ) <sub>12</sub> CH <sub>3</sub>	7.1856	C <sub>15</sub> H <sub>31</sub> C <sub>6</sub> H <sub>5</sub>
5.0000	(C <sub>6</sub> H <sub>4</sub> I) <sub>2</sub> C <sub>6</sub> H <sub>5</sub>	7.3474	C <sub>28</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
5.0930	[CH(OH)C <sub>6</sub> H <sub>5</sub> ] <sub>2</sub> •H <sub>2</sub> O	7.7475	C <sub>6</sub> H <sub>5</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>
5.0997	C <sub>12</sub> H <sub>25</sub> NH <sub>3</sub> Br	8.0176	C <sub>17</sub> H <sub>35</sub> C <sub>6</sub> H <sub>5</sub>
5.1010	C <sub>16</sub> H <sub>33</sub> S <sub>4</sub> Na•0.25H <sub>2</sub> O	8.0413	C <sub>10</sub> H <sub>7</sub> C <sub>6</sub> H <sub>5</sub>
5.1361	C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> NiO <sub>2</sub>	8.0433	C <sub>28</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>
5.1411	C <sub>16</sub> H <sub>8</sub> O <sub>2</sub> S <sub>2</sub>	8.0513	N <sub>6</sub> •C <sub>6</sub> H <sub>4</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>
5.1637	C <sub>7</sub> H <sub>4</sub> Cl <sub>2</sub> N <sub>4</sub>	8.0734	C <sub>17</sub> H <sub>35</sub> C <sub>6</sub> H <sub>5</sub>
5.1644	Pb(S <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	8.2530	C <sub>19</sub> H <sub>36</sub> O <sub>2</sub>
5.1675	C <sub>10</sub> H <sub>12</sub> Br <sub>2</sub> N <sub>2</sub>	8.2645	Br(CH <sub>2</sub> ) <sub>10</sub> C <sub>6</sub> H <sub>5</sub>
5.1786	C <sub>40</sub> H <sub>16</sub>	8.3123	Br•C <sub>6</sub> H <sub>4</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>
5.2690	C <sub>10</sub> H <sub>21</sub> C <sub>6</sub> H <sub>5</sub>	8.4625	Cl•C <sub>6</sub> H <sub>4</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>
5.2981	Cl-C <sub>6</sub> H <sub>4</sub> -CH-N <sub>2</sub> O	8.5654	C <sub>8</sub> H <sub>17</sub> CH:CH(CH <sub>2</sub> ) <sub>7</sub> •C <sub>6</sub> H <sub>5</sub>
5.3151	[(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>3</sub> ] <sub>4</sub> [C <sub>6</sub> H <sub>5</sub> •C•C•CH:CH•C <sub>6</sub> H <sub>5</sub> ] <sub>2</sub>	8.6588	C <sub>34</sub> H <sub>16</sub> O <sub>2</sub>
5.3607	C <sub>18</sub> H <sub>37</sub> S <sub>4</sub> Na•0.25H <sub>2</sub> O	8.6947	C <sub>19</sub> H <sub>36</sub> O <sub>2</sub>
5.4269	N <sub>6</sub> •C <sub>6</sub> H <sub>4</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>	9.1662	C <sub>21</sub> H <sub>15</sub> N <sub>3</sub>
5.5629	C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>	9.4626	C <sub>30</sub> H <sub>56</sub> Cl <sub>6</sub>
5.5714	(C <sub>6</sub> H <sub>5</sub> )CH=C(CN) <sub>2</sub>	9.4769	C <sub>30</sub> H <sub>56</sub> Cl <sub>6</sub>
5.5819	C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> H <sub>5</sub> I	9.7347	C <sub>22</sub> H <sub>44</sub> O <sub>2</sub>
5.5975	CH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> •CH:CH•C <sub>6</sub> H <sub>5</sub>	10.4929	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>15</sub> O(CH <sub>2</sub> ) <sub>15</sub> CH <sub>3</sub>
5.6049	C <sub>11</sub> H <sub>23</sub> C <sub>6</sub> H <sub>5</sub>	10.5071	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>15</sub> O•C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>14</sub> CH <sub>3</sub>
5.6593	Br(CH <sub>2</sub> ) <sub>10</sub> C <sub>6</sub> H <sub>5</sub>	10.6539	C <sub>24</sub> H <sub>48</sub> O <sub>2</sub>
5.6723	NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> OH•HCl	11.4441	C <sub>26</sub> H <sub>52</sub> O <sub>2</sub>
5.6751	NH <sub>2</sub> C <sub>6</sub> (CH <sub>2</sub> ) <sub>14</sub> CH <sub>3</sub>	14.3515	C <sub>27</sub> H <sub>56</sub> O
5.6954	C <sub>36</sub> H <sub>74</sub>	16.3605	C <sub>19</sub> H <sub>14</sub>

2  
mC2/c C<sub>2h</sub><sup>6</sup> No. 15Inorganic - 301  
Organic - 315

## Inorganic

0.4070	CaHAs <sub>4</sub> •2H <sub>2</sub> O	0.5583	K <sub>4</sub> Fe(CN) <sub>6</sub> •3H <sub>2</sub> O
0.4110	CaHP <sub>4</sub> •2H <sub>2</sub> O	0.5791	Si <sub>2</sub> O <sub>2</sub>
0.4145	Al <sub>5</sub> Ca <sub>4</sub> (OH) <sub>5</sub> (P <sub>4</sub> ) <sub>6</sub> •11H <sub>2</sub> O	0.6167	RbFeS <sub>2</sub>
0.4145	CaS <sub>4</sub> •2H <sub>2</sub> O	0.6197	KFeSe <sub>2</sub>
0.4202	CaSe <sub>4</sub> •2H <sub>2</sub> O	0.6221	RbFeSe <sub>2</sub>
0.4476	MgHP <sub>4</sub> •7H <sub>2</sub> O	0.6228	K <sub>3</sub> SnF <sub>6</sub> (HF <sub>2</sub> )
0.4881	YTa <sub>4</sub>	0.6250	KFeS <sub>2</sub>
0.5426	Fe <sub>2</sub> Mn(OH) <sub>2</sub> (P <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> O	0.6291	K <sub>3</sub> (HF <sub>2</sub> )(Nb <sub>2</sub> F <sub>5</sub> )
0.5536	K <sub>4</sub> Ru(CN) <sub>6</sub> •3H <sub>2</sub> O	0.6542	Sr(N <sub>3</sub> ) <sub>2</sub> •4H <sub>2</sub> O

C2/c  $C_{2h}^6$  No. 15 (continued)

## Inorganic (continued)

0.6589	$Al_2Ca(F,OH)_8$	1.0078	$FeSe_4 \cdot H_2O$
0.6595	$Al_2Ca(F,OH)_8$	1.0123	$BaAl_2Si_2O_8$
0.7027	$CsLiF_2$	1.0132	$MnSe_4 \cdot H_2O$
0.7043	$RbLiF_2$	1.0176	$MnSe_4 \cdot H_2O$
0.7366	$PbCl_5$	1.0185	$NdYb(WO_4)_3$
0.7523	$Ag_2PbO_2$	1.0192	$MnSe_4 \cdot H_2O$
0.7753	$Ca_3(WO_4)_2$	1.0209	$FeSe_4 \cdot H_2O$
0.7878	$AlCaH(Pb_4)_2 \cdot 6H_2O$	1.0265	$LiAsO_3$
0.7897	$CaMg(F,OH)Pb_4$	1.0298	CrS
0.7925	$K[AsF_4(OH)_2]$	1.0392	$NaVO_3$
0.8099	$Ba(SbO_3)_2 \cdot 8H_2O$	1.0437	$FeGeO_3$
0.8115	$CaTiO_3SiO_4$	1.0448	$(NH_3)_2Cl_4Pt$
0.8168	$RbBiO_2$	1.0476	$CoGeO_3$
0.8274	$AlNaF(AsO_4)$	1.0584	$(Mg,Fe)SiO_3$
0.8312	$NaB_5O_8 \cdot 5H_2O$	1.0598	$P_2P_4$
0.8394	$KBiO_2$	1.0625	$MgSiO_3$
0.8445	$BaPt(CN)_4 \cdot 4H_2O$	1.0672	$LiFeSi_2O_6$
0.8480	$H_2O_2 \cdot 2H_2O$	1.0707	$(Na,Ca)(Fe,Al,Mg,Fe)Si_2O_6$
0.8525	$Cu_2Mg_2(OH)_6CO_3 \cdot 2H_2O$	1.0723	$CoGeO_3$
0.8681	$(Fe,Mn)_2(Na,Ca)(Pb_4)_2$	1.0745	$CoGeO_3$
0.8684	$(Na,Ca,Fe,Mn)Pb_4$	1.0791	$NaCrSi_2O_6$
0.8717	$(Pb,Ca,Na,Mn)_3(Mg,Mn)_2(AsO_4)_{3-y}(OH)_x$	1.0795	$CoSe_4 \cdot 7H_2O$
0.8801	$(Fe,Mn)NaPb_4$	1.0814	$NiP_2$
0.8813	$SrO_2 \cdot 2H_2O$	1.0818	$(Ca_{0.32}Mg_{0.37}Fe_{0.31})SiO_3$
0.9059	$BaO_2 \cdot 2H_2O$	1.0818	$[CaFeSi_2O_6]$
0.9476	$NiSe_4 \cdot H_2O$	1.0847	$NaAlSi_2O_6$
0.9486	$CoSe_4 \cdot H_2O$	1.0871	$(Ca,Na)[Mg,Fe,Fe,Al](Si_2O_6)$
0.9493	$NiSe_4 \cdot H_2O$	1.0876	$CaMn(SiO_3)_2$
0.9520	$ZnSe_4 \cdot H_2O$	1.0877	$(Ca,Fe)(Mg,Fe)(Si,Al)_2O_6$
0.9560	$ZnSe_4 \cdot H_2O$	1.0877	$[Na,Ca,Mn,Fe,Fe,Al](Si,Al)_3O_3$
0.9564	$F_4O_8$	1.0878	$CaNiSi_2O_6$
0.9568	$ZnSe_4 \cdot H_2O$	1.0883	$NaAlSi_2O_6$
0.9572	$UF_4$	1.0885	$CaMg(SiO_3)_2$
0.9596	$ZrF_4$	1.0889	$CaMg(SiO_3)_2$
0.9619	$MnSe_4 \cdot H_2O$	1.0897	$CaMg(SiO_3)_2$
0.9623	$CeF_4$	1.0900	$(Na,Mg,Ca)(Mn,Fe)Si_2O_6$
0.9625	$HfF_4$	1.0900	$CaMg(SiO_3)_2$
0.9629	$UF_4$	1.0915	$Ca(Mg,Fe)Si_2O_6$
0.9636	$ThF_4$	1.0918	$Ca(Fe,Mg)(SiO_3)_2$
0.9665	$UF_4$	1.0920	$CaFe(SiO_3)_2$
0.9669	$PuF_4$	1.0941	$CaCo(SiO_3)_2$
0.9671	$NpF_4$	1.0980	$(K,Na)_{0.5}(Ca,Na,K)_2(Mg,Fe)_3(Fe,Al,Ti)_2$
0.9675	$TbF_4$		$Al_2Si_6O_{25}$
0.9743	$NiSe_4 \cdot H_2O$	1.0980	$Na_2ZrSi_4O_{11}$
0.9746	$NiSe_4 \cdot H_2O$	1.0980	AgCNS
0.9765	$NiSe_4 \cdot H_2O$	1.0988	$LiAlSi_2O_6$
0.9779	$MgSe_4 \cdot H_2O$	1.1050	$Li_2TiO_3$
0.9812	$MgSe_4 \cdot H_2O$	1.1093	$K_8Ta_6O_{19} \cdot 16H_2O$
0.9821	$Ce_2(WO_4)_3$	1.1311	$Na_2PbO_3$
0.9838	$LaY(WO_4)_3$	1.1315	$Cu_2P_2O_7$
0.9847	$LaYb(WO_4)_3$	1.1350	$Na_2B_4O_7 \cdot 10H_2O$
0.9848	$La_2(WO_4)_3$	1.1423	$Na_2ZrO_3$
0.9849	$CoSe_4 \cdot H_2O$	1.1427	$Na_2B_4O_7 \cdot 10H_2O$
0.9855	$CoSe_4 \cdot H_2O$	1.1470	$K_2ThO_3$
0.9863	$LaNd(WO_4)_3$	1.1532	$Na_2SnO_3$
0.9867	$Cr_2F_5$	1.1593	$Na_2B_4O_7 \cdot 10H_2O$
0.9879	$GdPr(WO_4)_3$	1.1622	$VS_4$
0.9893	$ZnSe_4 \cdot H_2O$	1.1987	$Ba(ClO_3)_2 \cdot H_2O$
0.9905	$CeEu(WO_4)_3$	1.2190	$CaNa_2(SO_4)_2$
0.9905	$CeY(WO_4)_3$	1.2197	$Ba(BrO_3)_2 \cdot H_2O$
0.9906	$ZnSe_4 \cdot H_2O$	1.2452	$3CdSO_4 \cdot 8H_2O$
0.9914	$Ce_2(WO_4)_3$	1.2938	$Nb_2ClO_4$
0.9918	$Na_4Se_4$	1.3101	$B_5H_8I$
0.9931	$Pr_2(WO_4)_3$	1.3214	$BaO_2 \cdot 2H_2O$
0.9931	$Nd_2(WO_4)_3$	1.3268	$K_4UO_2(CO_3)_3$
0.9939	$Tb_2(WO_4)_3$	1.3343	$MgUO_4$
0.9942	$Eu_2(WO_4)_3$	1.3347	$Be_3(Ca,Mn,Fe)_3(OH)_3(Pb_4)_3 \cdot 2H_2O$
0.9947	$Dy_2(WO_4)_3$	1.3715	$SrO_2 \cdot 2H_2O$
0.9956	$Sm_2(WO_4)_3$	1.3723	$(NH_4)_4UO_2(CO_3)_3$
0.9974	$Eu_2(WO_4)_3$	1.3727	$H_2O$
0.9974	$ZnSe_4 \cdot H_2O$	1.3928	$CdAl_4O_7$
0.9982	$Gd_2(WO_4)_3$	1.4009	$CaAl_4O_7$
1.0069	$FeSe_4 \cdot H_2O$	1.4029	$SrAl_4O_7$
1.0075	$(Cu,Fe,Zn)Se_4 \cdot H_2O$	1.4056	$CaAl_4O_7$

C2/c C<sub>2h</sub><sup>6</sup> No. 15 (continued)

## Inorganic (continued)

1.4166	Na <sub>2</sub> Cd <sub>3</sub> •10H <sub>2</sub> O	2.3910	Ca[B(OH) <sub>4</sub> ] <sub>2</sub> •2H <sub>2</sub> O
1.4391	Nd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> •5H <sub>2</sub> O	2.3967	Ca <sub>3</sub> Na <sub>2</sub> (OH) <sub>2</sub> Cl(SO <sub>4</sub> ) <sub>2</sub> B <sub>5</sub> O <sub>8</sub>
1.4421	Pr <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> •5H <sub>2</sub> O	2.4118	Na <sub>4</sub> P <sub>2</sub> O <sub>7</sub> •10H <sub>2</sub> O
1.4795	Pb(SCN) <sub>2</sub>	2.4368	Na <sub>4</sub> P <sub>2</sub> O <sub>7</sub> •10H <sub>2</sub> O
1.4900	Na <sub>2</sub> Ca(CO <sub>3</sub> ) <sub>2</sub> •5H <sub>2</sub> O	2.4395	Zn <sub>2</sub> Te <sub>3</sub> O <sub>8</sub>
1.4979	CuO	2.4628	Sb <sub>2</sub> O <sub>4</sub>
1.5472	ThC <sub>2</sub>	2.4814	Mn <sub>14</sub> Na <sub>6</sub> H <sub>2</sub> (PO <sub>4</sub> ) <sub>12</sub> •H <sub>2</sub> O
1.5922	Th(OH) <sub>2</sub> (NO <sub>3</sub> ) <sub>2</sub> •xH <sub>2</sub> O	2.5285	C <sub>2</sub> Fe <sub>5</sub>
1.6014	B <sub>3</sub> N <sub>14</sub>	2.5497	C <sub>2</sub> Mn <sub>5</sub>
1.6215	Al <sub>2</sub> Ca <sub>3</sub> F <sub>4</sub> (OH, F) <sub>6</sub> SO <sub>4</sub> •2H <sub>2</sub> O	2.5605	Nb <sub>2</sub> O <sub>5</sub>
1.6220	Li <sub>2</sub> CO <sub>3</sub>	2.5617	CaMg[B <sub>3</sub> O <sub>3</sub> (OH) <sub>5</sub> ] <sub>2</sub> •6H <sub>2</sub> O
1.6275	2HgSO <sub>4</sub> •HgO•2H <sub>2</sub> O	2.5813	SrS <sub>2</sub> O <sub>3</sub> •5H <sub>2</sub> O
1.6409	Nd <sub>2</sub> NE <sub>2</sub>	2.5975	K <sub>4</sub> [Te <sub>2</sub> O <sub>6</sub> (OH) <sub>4</sub> ](H <sub>2</sub> O) <sub>7.3</sub>
1.6529	Co(AlCl <sub>4</sub> ) <sub>2</sub>	2.6187	NH <sub>4</sub> B <sub>5</sub> O <sub>8</sub> •8/3H <sub>2</sub> O
1.6667	K <sub>2</sub> NH(SO <sub>3</sub> ) <sub>2</sub>	2.6643	Ca(H <sub>2</sub> PO <sub>4</sub> ) <sub>2</sub>
1.6760	Ca <sub>8</sub> FeOH(PO <sub>4</sub> ) <sub>6</sub> •10H <sub>2</sub> O	2.6677	Ca <sub>5</sub> K <sub>2</sub> (SO <sub>4</sub> ) <sub>6</sub> •H <sub>2</sub> O
1.6777	AlCu <sub>2</sub> (OH) <sub>4</sub> (As, P) <sub>4</sub> •4H <sub>2</sub> O	2.6698	MnF <sub>3</sub>
1.6790	K <sub>2</sub> PaF <sub>7</sub>	2.6838	Pr <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> •8H <sub>2</sub> O
1.6826	AgO	2.6956	Nd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> •8H <sub>2</sub> O
1.6895	K <sub>2</sub> S <sub>2</sub> O <sub>7</sub>	2.6990	NH <sub>2</sub> NE <sub>2</sub> •HBF <sub>4</sub>
1.7586	(NB <sub>4</sub> ) <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>	2.7071	Sm <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> •8H <sub>2</sub> O
1.7597	SnCl <sub>4</sub> •2SeO <sub>2</sub> Cl <sub>2</sub>	2.7126	Sm <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> •8H <sub>2</sub> O
1.7621	[Cr(H <sub>2</sub> O) <sub>4</sub> Cl <sub>2</sub> ] <sub>2</sub> Cl•2H <sub>2</sub> O	2.7343	Ag <sub>3</sub> AsS <sub>3</sub>
1.7665	FeC <sub>2</sub> O <sub>4</sub> •2H <sub>2</sub> O	2.8041	CaSb <sub>2</sub> F <sub>7</sub>
1.7718	Tl <sub>2</sub> S <sub>3</sub> O <sub>6</sub>	2.8171	SnF <sub>2</sub>
1.7720	K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>	2.8304	N <sub>2</sub> H <sub>5</sub> Br
1.7924	[Co(NH <sub>3</sub> ) <sub>6</sub> ] <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> •5H <sub>2</sub> O	2.9189	(Mn, Zn, Mg) <sub>7</sub> (CO <sub>3</sub> ) <sub>2</sub> (OH) <sub>10</sub>
1.7986	K <sub>2</sub> Mo <sub>3</sub> O <sub>10</sub>	2.9571	LiAlSi <sub>4</sub> O <sub>10</sub>
1.8153	NaSi	3.0000	AgSbS <sub>2</sub>
1.8170	H <sub>2</sub> SO <sub>4</sub>	3.0534	Na <sub>5</sub> P <sub>3</sub> O <sub>10</sub>
1.8619	Fe <sub>7</sub> S <sub>8</sub>	3.0748	Al <sub>2</sub> Mg <sub>5</sub> Si <sub>3</sub> O <sub>10</sub> (OH) <sub>8</sub>
1.8743	BaS <sub>2</sub> O <sub>6</sub> •2H <sub>2</sub> O	3.0869	(Mg, Fe) <sub>3</sub> (OH) <sub>2</sub> (Si, Al, Fe) <sub>4</sub> O <sub>10</sub> •4H <sub>2</sub> O
1.8961	NaBeSi <sub>3</sub> O <sub>7</sub> (OH)	3.0975	(Mg, Al, Fe) <sub>6</sub> Si <sub>3</sub> AlO <sub>10</sub> (OH) <sub>8</sub>
1.9001	Ca <sub>5</sub> H <sub>2</sub> (AsO <sub>4</sub> ) <sub>4</sub> •4H <sub>2</sub> O	3.1034	[Mg, Fe, Al] <sub>3</sub> (Si, Al) <sub>4</sub> O <sub>10</sub> (OH) <sub>2</sub> (Mg <sub>1-x</sub> H <sub>2</sub> O <sub>6-y</sub> )
1.9087	NaBeSi <sub>3</sub> O <sub>7</sub> (OH)	3.1189	(Mg, Fe) <sub>3</sub> (Si, Al) <sub>4</sub> O <sub>9</sub> (OH) <sub>2</sub> •4H <sub>2</sub> O
2.0071	Na <sub>2</sub> H <sub>2</sub> P <sub>2</sub> O <sub>7</sub> •6H <sub>2</sub> O	3.1315	(Mg, Al, Fe) <sub>5</sub> Al <sub>2</sub> Si <sub>3</sub> O <sub>10</sub> (OH) <sub>8</sub>
2.0118	Hg <sub>4</sub> O <sub>2</sub> Cl <sub>2</sub>	3.1896	Na <sub>2</sub> CeO <sub>3</sub>
2.0171	Na <sub>2</sub> H <sub>2</sub> P <sub>2</sub> O <sub>7</sub> •6H <sub>2</sub> O	3.2068	Na <sub>2</sub> PrO <sub>3</sub>
2.0450	Pb <sub>9</sub> Sb <sub>8</sub> S <sub>21</sub>	3.2138	Li <sub>2</sub> PtO <sub>3</sub>
2.0473	Mg <sub>3</sub> Si <sub>4</sub> O <sub>10</sub> (OH) <sub>2</sub>	3.2220	Li <sub>2</sub> SnO <sub>3</sub>
2.0608	Al <sub>2</sub> (OH) <sub>2</sub> (Si <sub>2</sub> O <sub>5</sub> ) <sub>2</sub>	3.2284	K <sub>5</sub> (UO <sub>2</sub> ) <sub>2</sub> F <sub>9</sub>
2.0611	N <sub>2</sub> H <sub>5</sub> ClO <sub>4</sub> •0.5H <sub>2</sub> O	3.2354	Li <sub>2</sub> RhO <sub>3</sub>
2.0652	Al <sub>2</sub> Si <sub>4</sub> O <sub>10</sub> (OH) <sub>2</sub>	3.2613	Li <sub>2</sub> IrO <sub>3</sub>
2.0773	OsO <sub>4</sub>	3.2648	Li <sub>2</sub> TiO <sub>3</sub>
2.0792	Ca(Mg, Al, Ca) <sub>3</sub> (Al, Si) <sub>4</sub> O <sub>10</sub> (OH) <sub>2</sub>	3.2904	Li <sub>2</sub> PdO <sub>3</sub>
2.0836	Na <sub>3</sub> TaF <sub>8</sub>	3.3024	K <sub>2</sub> Cd(SCN) <sub>4</sub> •2H <sub>2</sub> O
2.1359	(NH <sub>4</sub> ) <sub>6</sub> TeMo <sub>6</sub> O <sub>24</sub> •H <sub>6</sub> TeO <sub>6</sub> •7H <sub>2</sub> O	3.3254	(Al, Fe)(Fe, Mg)(OH) <sub>2</sub> AlSi <sub>6</sub> O <sub>5</sub>
2.1542	Al <sub>2</sub> Ca(OH) <sub>2</sub> Al <sub>2</sub> Si <sub>2</sub> O <sub>10</sub>	3.3473	NiSO <sub>4</sub> •6H <sub>2</sub> O
2.1615	CaAl <sub>2</sub> (Li, H)(OH) <sub>2</sub> AlBeSi <sub>2</sub> O <sub>10</sub>	3.3542	CoSO <sub>4</sub> •6H <sub>2</sub> O
2.1631	Al <sub>2</sub> Ca(OH) <sub>2</sub> (Al, Si) <sub>4</sub> O <sub>10</sub>	3.3728	MgSeO <sub>4</sub> •6H <sub>2</sub> O
2.1774	Al <sub>2</sub> Ca(OH) <sub>2</sub> (Al <sub>2</sub> Si <sub>2</sub> O <sub>10</sub> )	3.3750	CoSO <sub>4</sub> •6H <sub>2</sub> O
2.1788	K(Mg, Fe, Mn) <sub>3</sub> (OH, F) <sub>2</sub> AlSi <sub>3</sub> O <sub>10</sub>	3.3763	Na <sub>2</sub> ZrO <sub>3</sub>
2.1896	K(Fe, Mg) <sub>3</sub> (Si, Al) <sub>4</sub> O <sub>10</sub> (OH) <sub>2</sub>	3.3846	MgSO <sub>4</sub> •6H <sub>2</sub> O
2.1949	KMg <sub>3</sub> AlSi <sub>3</sub> O <sub>10</sub> (OH) <sub>2</sub>	3.3859	Na <sub>2</sub> IrO <sub>3</sub>
2.1957	KMg <sub>3</sub> (OH, F) <sub>2</sub> (Al, Si) <sub>4</sub> O <sub>10</sub>	3.3908	Na <sub>2</sub> PtO <sub>3</sub>
2.1961	KMg <sub>2</sub> B <sub>11</sub> O <sub>19</sub> •15H <sub>2</sub> O	3.4011	MgSeO <sub>4</sub> •6H <sub>2</sub> O
2.2115	(K, Na, Ca)(Al, Cr, Fe, Mg) <sub>2</sub> (OH) <sub>2</sub> (AlSi <sub>3</sub> )O <sub>10</sub>	3.4042	MgSO <sub>4</sub> •6H <sub>2</sub> O
2.2165	AgAsS <sub>2</sub>	3.4082	Cu(NO <sub>3</sub> ) <sub>2</sub> •1.5H <sub>2</sub> O
2.2217	KAl <sub>2</sub> (AlSi <sub>3</sub> )O <sub>10</sub> (OH) <sub>2</sub>	3.4294	Li <sub>2</sub> TcO <sub>3</sub>
2.2258	KAl <sub>2</sub> (OH) <sub>2</sub> AlSi <sub>3</sub> O <sub>10</sub>	3.4513	Na <sub>5</sub> P <sub>3</sub> O <sub>10</sub>
2.2278	V(OH) <sub>2</sub>	3.4681	Li <sub>2</sub> MoO <sub>3</sub>
2.2371	KAl <sub>2</sub> (AlSi <sub>3</sub> )O <sub>10</sub> (OH) <sub>2</sub>	3.4820	Hg(SCN) <sub>2</sub> Nl(NCS) <sub>2</sub> •2H <sub>2</sub> O
2.2433	Al <sub>2</sub> K(OH) <sub>2</sub> (AlSi <sub>3</sub> O <sub>10</sub> )	3.5278	Sn(Ta, Nb) <sub>2</sub> O <sub>7</sub>
2.2497	KAl <sub>2</sub> (OH) <sub>2</sub> AlSi <sub>3</sub> O <sub>10</sub>	3.7655	NaHSeO <sub>3</sub>
2.3167	K <sub>2</sub> H <sub>2</sub> P <sub>2</sub> O <sub>7</sub> •0.5H <sub>2</sub> O	4.0253	FeFe <sub>5</sub> (OH) <sub>5</sub> (PO <sub>4</sub> ) <sub>4</sub> •6H <sub>2</sub> O
2.3192	Zr <sub>2</sub> (OH) <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> •4H <sub>2</sub> O	5.7622	Na <sub>3</sub> H(CO <sub>3</sub> ) <sub>2</sub> •2H <sub>2</sub> O
2.3284	Co(NO <sub>3</sub> ) <sub>2</sub> •6H <sub>2</sub> O	7.5625	HgSb <sub>4</sub> S <sub>8</sub>
2.3773	Al(UO <sub>2</sub> ) <sub>2</sub> (OH)(VO <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> O	7.8486	Nb <sub>12</sub> O <sub>29</sub>



C2/c  $C_{2h}^6$  No. 15 (continued)

## Organic

0.2046	$Cu(C_6H_5COO)_2 \cdot 3H_2O$	1.4272	$(CH_2)_2 \cdot C_6H_5$
0.4424	$C_6H_8O_2 \cdot HgCl_2$	1.4307	$C_{12}H_8Cl_2$
0.5515	$C_7H_{12}O_4$	1.4366	$(CH_3)_2NC_6H_4N_2Cl_2 \cdot ZnCl_2$
0.5536	$K_4Ru(CN)_6 \cdot 3H_2O$	1.4480	$C_6(NH_2)_6$
0.5583	$K_4Fe(CN)_6 \cdot 3H_2O$	1.4761	$C_6H_8Cl_4$
0.5588	$C_6H_5C_2AgP(CH_3)_3$	1.4771	$C_{10}H_8Br_4$
0.6260	$CuCl_2 \cdot C_2N_3H_3$	1.4795	$Pb(SCN)_2$
0.6706	$C_6H_4(COOH)_2$	1.4900	$Na_2Ca(CO_3)_2 \cdot 5H_2O$
0.6906	$C_8H_{12}N_2O_3$	1.5094	$C_3N_3Cl_3$
0.7009	$LiCl \cdot (NH_2CH_2CH_2NH_2)_2$	1.5107	$Pd(SCN_2H_4)_4Cl_2$
0.7064	$[(C_6H_5)_3O]Cl \cdot 2H_2O$	1.5472	$ThC_2$
0.7080	$[(C_6H_5)_3O]Br \cdot 2H_2O$	1.5541	$Na \cdot UO_2(C_6H_5NO)_3$
0.7222	$C_{14}H_{10} \cdot C_6H_3(NH_2)_3$	1.5752	$3(CH_6ClN_3) \cdot CH_3CO_2N(CH_3)_2$
0.7244	$Cu(C_3H_7O)_2 \cdot C_5H_5N$	1.5792	$C_{22}H_{28}O_{16}$
0.7578	$2[(CH_3)_2NOC_6H_4 \cdot I] \cdot HCl \cdot HI \cdot I_2$	1.6041	$C_6NH_2(CH_2)_3C_6NH_2$
0.7692	$Ba(C_4H_{10}PO_4)_2$	1.6153	$K_2[CH_2(SO_3)_2]$
0.7711	$CH_3O \cdot C_6H_4 \cdot CH : CH \cdot COOH$	1.6169	$C_6H_3(COOH)_3$
0.7786	$2((CH_3)_2N-C_6H_4-N_2) \cdot (ZnCl_4)$	1.6178	$CH_2(SO_3NH_4)_2$
0.7801	$C_6H_5Br_3N_2$	1.6194	$CH_2(SO_3K)_2$
0.8080	$(C_6H_5)_2COH(C_6H_2Br_2OH)$	1.6220	$Li_2CO_3$
0.8186	$C_6H_4N_4O_4$	1.6304	$Cr_2(CH_3CO_2)_4 \cdot 2H_2O$
0.8444	$Cl \cdot CH_2 \cdot CO_2NH_4$	1.6315	$Cu_2(CH_3COO)_4 \cdot 2H_2O$
0.8445	$BaPt(CN)_4 \cdot 4H_2O$	1.6355	$(C_6H_5CH_2S)_2$
0.8561	$I \cdot C_6H_4 \cdot CN$	1.6364	$(CH_3)_2CO \cdot Br_2$
0.8577	$Zn(C_6H_5N_3O)_2 \cdot 5H_2O$	1.6450	$Rb_2C_2O_4 \cdot H_2O$
0.9048	$RbH(CF_3COO)_2$	1.6524	$(C_6H_5CH_2Se)_2$
0.9072	$KH(CF_3COO)_2$	1.6589	$Co(C_5H_{10}NS_2)_3$
0.9121	$(CH_3)_2NC_6H_4 \cdot NH \cdot C_6H_4N(CH_3)_2 \cdot I$	1.6771	$K_2C_2O_4 \cdot H_2O$
0.9190	$K_2C_6O_6$	1.6790	$(CH_3)_2NH_2CuCl_3$
0.9196	$Te(C_4H_8N_2S)_2(SCN)_2$	1.6885	$C_{12}H_{18}$
0.9211	$NaHCO_2$	1.7020	$V(C_{14}H_{10}S_2)_3$
0.9345	$[(CH_3)_2N]_2C \cdot S$	1.7151	$C_{22}H_{32}O_2$
0.9592	$Te_7(C_3H_6N_2S)_{12}Br_{16}$	1.7221	$Fe(CO)_5$
0.9782	$UO_2Br_2 \cdot 3[(CH_3)_2N \cdot COOH]$	1.7232	$C_6H_4As_2Cl_2O$
0.9816	$C_4H_{12}I_5N$	1.7232	$LiNH_4C_4H_4O_6 \cdot H_2O$
0.9890	$Cl_2(C_6H_5)_4P_3N_3$	1.7291	$(COOK)_2 \cdot H_2O$
0.9965	$(CH_3)_2C_5H_3N \cdot CO(NH_2)_2$	1.7382	$Rh_6(CO)_{16}$
1.0122	$Ag(H_2NCSNH_2)_2SCN$	1.7461	$Rb_2C_2O_4 \cdot H_2O$
1.0344	$Se[(C_2H_5)_2PSe_2]_2$	1.7513	$K_2Ni(CO)_4$
1.0475	$C_6H_8O_4S_2$	1.7665	$FeC_2O_4 \cdot 2H_2O$
1.0566	$Te[(C_2H_5)_2PSe_2]_2$	1.7763	$K_2Pd(CO)_4$
1.0573	$C_6H_8O_4Se_2$	1.8072	$C_4H_8SeBr_2$
1.0627	$C_5H_{10}H_3O_3$	1.8107	$(AlCl_2CH_3)_2$
1.0980	$AgCNS$	1.8178	$K_2Pt(CO)_4$
1.1139	$(C_4H_4NO)_2$	1.8320	$SbI_3 \cdot 2C_4H_8S_2$
1.1262	$ZnCl_2 \cdot 2C_7H_8O_2$	1.8419	$Rb(SbO)_4C_4H_4O_6 \cdot H_2O$
1.1504	$Ru(CO)_4I_2$	1.8504	$(NH_2CSNH_2)_2TeCl_2$
1.1527	$C_{26}H_{16}O_2$	1.8504	$C_{18}H_{16}CdCl_4N_2$
1.1783	$Co[N(CH_3)_5]_4(NCS)_2$	1.8678	$[(CH_3)_3Al]_2$
1.1819	$CH_3COONa \cdot 3H_2O$	1.8911	$C_6H_{10}(OH)_2$
1.1910	$[(CH_3)_2NCS]_2S_2$	1.8915	$K[(CH_3) \cdot CO \cdot CH \cdot C(CH_3)O]_2PtCl$
1.2064	$Pd(C_{10}H_8N_3)_2$	1.8939	$C_{10}Cl_8$
1.2180	$C_4K_2O_4 \cdot H_2O$	1.8953	$(NH_2CSNH_2)_2TeBr_2$
1.2357	$(CH_2CO_2NH_2)_2$	1.9094	$Cd[SC(NHCH_2)_2]_2(NCS)_2$
1.2414	$H_2O \cdot C_8H_{14} \cdot COOH$	1.9128	$NH_4(SbO)_4C_4H_4O_6 \cdot H_2O$
1.2528	$CH_3N_2OK$	1.9433	$2(CH_3)_2NCOCH_3 \cdot NaClO_4$
1.2538	$B_{10}H_{12}(CH_3CN)_2$	1.9504	$[(C_2H_5)_3PtCl]_4$
1.2596	$Na_3C_6H_5O_7 \cdot 2H_2O$	2.0051	$Te(C_4H_8N_2S)_2Br_2$
1.2636	$(CH_3)_2C(NH_2)COOH$	2.0128	$C_{23}H_{16}IN_6$
1.3056	$C_{10}H_8Cl_4$	2.0200	$NH_2CO(CH_2)_5CO_2NH_2$
1.3292	$Ti(O_2C_2H_5)_4$	2.0202	$(C_4H_9)_4Nc(C_4N_2S_2)_2$
1.3307	$Co(C_5H_7O)_2 \cdot H_2O$	2.0314	$C_5H_5NH[Cr(NCS)_4(NH_3)_2]$
1.3412	$(HCNO)_3$	2.0419	$Te(C_4H_8N_2S)_2Cl_2$
1.3451	$[NH_2C_6H_4C_6H_4NH_2][Cr(NCS)_4(NH_3)_2]_2$	2.0466	$Pb[SC(NHCH_2)_2]_2(NCS)_2$
1.3573	$C_6H_8CuNaN_3O_4 \cdot H_2O$	2.0633	$Mn_2(CO)_{10}$
1.3602	$C_{14}H_8O_2$	2.0697	$(As(C_6H_5)_4)_2Co(NH_3)_4$
1.3643	$C_{18}H_{20}$	2.0754	$U(CH_3COO)_4$
1.3723	$(NH_4)_4UO_2(CO_3)_3$	2.0794	$Tc_2(CO)_{10}$
1.3837	$Mo(CO)_4[(C_6H_5)_3PO]_2$	2.0853	$Re_2(CO)_{10}$
1.3864	$C_8H_{10}$	2.1041	$C_{30}H_{44}O_{16}$
1.3953	$C_{30}H_{18}Cl_2$	2.1293	$C_4H_{10}N_2 \cdot 2HCl \cdot H_2O$
1.4129	$Co_2(CO)_4(C_2H_2)(C_4H_9 \cdot C \cdot CH)_2$	2.1520	$C_{20}H_{22}O_{16}$
1.4166	$Na_2CO_3 \cdot 10H_2O$	2.1662	$(C_2H_5C_5H_4FeC_5H_4)_2$

C2/c  $C_{2h}^6$  No. 15 (continued)

## Organic (continued)

2.1708	$C_{10}H_6(N_2)_2$	3.4789	$C_9H_{13}N_5 \cdot HCl$
2.1800	$[(C_5H_5)_2Ti]Cl_2$	3.4820	$Hg(SCN)_2Ni(NCS)_2 \cdot 2H_2O$
2.1899	$Cl_2BeC_2H_4 \cdot HCl_2$	3.5106	$C_{18}H_{16}O_6$
2.2099	$C_{12}H_8N_2O_2$	3.5212	$C_{12}H_{10}N_2O_2$
2.2112	$C_{12}H_{24}Br_2N_8S_4Te$	3.5215	$(C_6H_5)_2I \cdot I$
2.2557	$C_6H_{10}O_4$	3.5376	$C_{30}H_{36}O_4$
2.3040	$C_6H_{12}Br_2N_4S_2Te$	3.5756	$(C_6H_5)_2I \cdot Cl$
2.3089	$C_6H_{11}NO$	3.5898	$[(CH_3)_3PtC_5H_7O_2]_2NH_2CH_2CH_2NH_2$
2.3137	$C_7H_9NCr(CO)_3$	3.6135	$H_6OC(CH_2)_5COOH$
2.3222	$C_{12}H_4N_4$	3.6247	$C_{10}H_{12}N_2O \cdot C_4H_7N_3O \cdot H_2SO_4 \cdot H_2O$
2.3346	$C_8H_{15}N_2SO \cdot HCl$	3.6585	$C_{10}H_6Cl_2$
2.3699	$Zr(CH_3CO \cdot CH : CO \cdot CH_3)_4$	3.6764	$C_{18}H_{12}$
2.3897	$Th(C_5H_7O)_4$	3.7122	$Ni(NH_2CSNHNH_2)_2 \cdot SO_4$
2.4086	$NH_2CO(CH_2)_7CONH_2$	3.7264	$Te(C_3H_6N_2S)_2(S_2O_2CH_3)_2$
2.4178	$IC_6H_5SO_2 \cdot C_4H_6NO$	3.8152	$C_6H_5 \cdot CH : CBr \cdot COOH$
2.4398	$C_6H_6O_2 \cdot (CH_3)_2CO$	3.8295	$(CH_3)_6C_6H_4 \cdot CH_2)_2$
2.4479	$(C_5H_5FeS)_4$	3.8312	$C_{16}H_{14}CuN_2O_2$
2.4839	$C_6H_5 \cdot C(:NOH) \cdot CO(:NOH) \cdot C_6H_5$	3.8500	$CH_2N_2 \cdot CH_2COOH$
2.5147	$C_{12}Cl_{12}$	3.8829	$Ca(C_{14}H_{18}N_2O_8 \cdot FeH_2O)_2 \cdot 8H_2O$
2.5285	$Fe_5C_2$	3.9081	$C_8H_{16}H_2O_2$
2.5497	$C_2Mn_5$	3.9235	$C_{28}H_{16}$
2.5504	$Pt(NH_3)_2[CH_3CO \cdot (NH_2)NH]_2Cl_2 \cdot H_2O$	4.0000	$C_{12}H_8I_2O_2S$
2.5534	$(C_6H_2Cl_3)_2$	4.0016	$Cu(C_6H_5CO \cdot CH \cdot CO \cdot C_6H_5)_2$
2.5729	$(C_2H_4COOH)_2(NH_2 \cdot (CH_2)_2)_2$	4.0335	$(Cl_2C_6H_4)_2SO_2$
2.6362	$Fe(C_8H_9)_2$	4.0344	$(ClC_6H_4)_2CO$
2.6495	$AgSCN \cdot [(C_6H_{11})_3P]_2$	4.0611	$Pd(C_6H_5CO \cdot CH \cdot CO \cdot C_6H_5)_2$
2.6530	$C_5H_8O_4$	4.1171	$(C_6H_4Br)_2SO_2$
2.6600	$C_{12}H_8N_4$	4.1804	$CH_3AsI_2$
2.6811	$(C_3H_8N_2S)_2TeI_2$	4.1987	$(C_7H_{11}O)_2Cu$
2.6811	$C_6H_{12}I_2N_4S_2Te$	4.2097	$(BrC_6H_4)_2Se$
2.7256	$Zn(CH_3COO)_2 \cdot 2H_2O$	4.2249	$H_6OC_6H_4 \cdot CONH_2$
2.7385	$Zn[PC_2(O_2C_2H_5)_2]_2$	4.2252	$(C_6H_5OHCl)_2CH_2$
2.7424	$B_{10}Br_3H_7C_2H_2$	4.2268	$N_6C_2C_6H_4COOH$
2.7637	$C_4H_3S \cdot COOH$	4.2338	$(BrC_6H_4)_2S$
2.7646	$Mg[(C_2H_5O)_2PO]_2$	4.2443	$Fe_3(CO)_8(C_6H_5C_2C_6H_5)_2$
2.7805	$Mg[PO_2(O_2C_2H_5)_2]_2$	4.2768	$(C_6H_5)_2C_2 \cdot Fe_2(CO)_8$
2.7858	$C_4H_8N_4O_4Ni \cdot 2H_2O$	4.2799	$C_{12}H_{10}N_3Cu$
2.7996	$C_2H_2N_2SO_2$	4.3651	$C_2H_5O \cdot C_6H_4 \cdot CH : CH \cdot COOH$
2.8014	$C_6H_{12}Br_2N_4S_2Te$	4.3736	$C_{32}H_{16}$
2.8057	$Cd(NH_2CH_2CO)_2 \cdot 2H_2O$	4.4448	$C_{30}H_{26}Fe_3$
2.8148	$NH_2CO \cdot (CH_2)_6 \cdot CONH_2$	4.4519	$C_7H_{10}O_4S_2$
2.8182	$Te(CSN_2H_4)_4(HF)_2$	4.4638	$Cu(C_6H_6NO)_2 \cdot 2(N_3C_6H_2(NO_2)_3)$
2.8415	$Co_4(CO)_{10}(C_2H_5C_2C_2H_5)$	4.5404	$C_6H_5 \cdot C(CN) : C(CN) \cdot C_6H_5$
2.8541	$C_{26}H_{23}O_2PS$	4.5664	$C_{10}H_6(C_6H_{11})_2$
2.8617	$[CH_2 \cdot NO \cdot (CH_2COOH)_2]_2$	4.5979	$(C_6H_5)_3Bi$
2.8768	$C_{12}H_{10}O_4S_3$	4.6135	$C_{14}H_{10}N_2S$
2.8821	$Se(SO_2C_6H_5)_2$	4.6263	$Bi(C_6H_5)_3$
2.9189	$(Mn, Zn, Mg)_7(CO_3)_2(OH)_{10}$	4.6914	$C_{14}H_8Cl_2$
2.9251	$(CF_3)_4C_5O \cdot C_5H_5 \cdot CO$	4.7025	$C_6H_4NO_2 \cdot OK \cdot 0.5H_2O$
2.9273	$C_{22}H_{14}$	4.7165	$C_{16}H_8Cl_2$
2.9289	$C_8H(CF_3COO)_2$	4.7294	$C_6H_4NO_2 \cdot OK \cdot 0.5H_2O$
2.9474	$C_8H_4O_4$	4.8837	$Br \cdot (CH_3O) \cdot C_6H_5 \cdot CH : CH \cdot COOH$
2.9943	$(ClHC:CH)_3SbCl_2$	4.8871	$(CH_3CO \cdot NH)_2C_3HS_2I$
3.0236	$Mn(CO)_5H$	5.0099	$BrC_6H_4N_2CONH_2$
3.0240	$C_{26}H_{16}O_2$	5.0124	$CH_3 \cdot (CH)_4 \cdot COOH$
3.0294	$(C_6H_5)_3P \cdot Fe_3(CO)_{11}$	5.0335	$(CH_2)_3(COOH)_2$
3.0301	$C_3H_6N_4O_3$	5.0433	$C_7H_9BrN_2O_2S_2$
3.0496	$(CH_3C_6H_4SO_2)_2S$	5.1782	$C_{10}H_{13}ClNO$
3.0529	$C_{17}H_{10}BrNS_2$	5.3333	$C_6H_2O_4 \cdot 2H_2O$
3.0963	$C_{14}H_{15}BrO_3S$	5.3842	$Fe(C_5H_4COOHCH_3)_2$
3.1114	$(CH)_2O(COOH)_2$	5.6000	$Br \cdot C_6H_4 \cdot COOH$
3.1506	$Ni(NH_2CH_2CH_2NH_2)_2(NCS)NO_2$	5.7622	$Na_3H(CO_3)_2 \cdot 2H_2O$
3.1786	$C_6H_{10}ClCuN_3O_4 \cdot 1.5H_2O$	5.9047	$C_6Cl_5OH$
3.1788	$Se(CH_3 \cdot C_6H_4 \cdot SO_2)_2$	6.0018	$C_{10}H_{19}NH_2 \cdot HCl \cdot 1.5H_2O$
3.2168	$(OC_6H_4CH=NC_6H_5)_2Cu \cdot C_5H_5N$	6.1641	$C_7H_5O_2Cl$
3.2257	$(PtCl \cdot CH_3 \cdot C_{10}H_{12})_2$	6.1796	$Br \cdot C_6H_4 \cdot CH : CH \cdot COOH$
3.2709	$C_{20}H_{14}$	6.2285	$C_{26}H_{14}N_8Ni$
3.3024	$K_2Cd(SCN)_4 \cdot 2H_2O$	6.2678	$C_5H_{11}NO_2$
3.3424	$(NH_4)_2C_6Cl_2O_4 \cdot H_2O$	6.3111	$(C_6H_5CH_2COO)_2KH$
3.3504	$Fe_5(CO)_{15}C$	6.3181	$C_{16}H_{15}O_4Rb$
3.3784	$C_2N_4H_4$	6.4846	$(C_6H_5 \cdot CH : CH \cdot COO)_2HNH_4$
3.4381	$C_{11}H_{10} \cdot Cr(CO)_3$	6.4925	$Br \cdot (CH_3O) \cdot C_6H_5 \cdot CH : CH \cdot COOH$
3.4424	$C_2H_3N_3S_2 \cdot HCl \cdot 0.5H_2O$	6.5428	$C_6H_2CH_3(NO_2)_3$
3.4510	$(C_6H_5)_2As \cdot C \cdot As(C_6H_5)_2$	6.6811	$Cl \cdot (CH_3O) \cdot C_6H_5 \cdot CH : CH \cdot COOH$

C<sub>2</sub>/c C<sub>2h</sub><sup>6</sup> No. 15 (continued)

## Organic (continued)

6.8106	CH <sub>3</sub> SCH <sub>2</sub> CH <sub>2</sub> CH(NH <sub>2</sub> )C <sub>6</sub> H <sub>5</sub>	9.6015	C <sub>6</sub> H <sub>4</sub> (CH <sub>2</sub> ) <sub>10</sub> NH <sub>2</sub> •HBr•0.5H <sub>2</sub> O
7.1182	C <sub>15</sub> H <sub>16</sub> NCl	9.9098	C <sub>6</sub> H <sub>13</sub> C <sub>6</sub> NH <sub>2</sub>
7.3137	[C <sub>18</sub> H <sub>16</sub> HgN <sub>2</sub> S <sub>2</sub> ]	10.9795	C <sub>7</sub> H <sub>15</sub> C <sub>6</sub> NH <sub>2</sub>
7.5828	C <sub>13</sub> H <sub>6</sub> N <sub>2</sub> S	12.0205	C <sub>8</sub> H <sub>17</sub> C <sub>6</sub> NH <sub>2</sub>
7.6000	HgCl <sub>2</sub> (C <sub>12</sub> H <sub>8</sub> S) <sub>2</sub>	12.9877	C <sub>17</sub> H <sub>35</sub> C <sub>6</sub> CH <sub>3</sub>
7.6108	KH(C <sub>6</sub> H <sub>5</sub> C <sub>6</sub> ) <sub>2</sub>	14.0667	[Br(CH <sub>2</sub> ) <sub>10</sub> C <sub>6</sub> ] <sub>2</sub> C <sub>3</sub> H <sub>7</sub>
8.2765	C <sub>20</sub> H <sub>18</sub> Cl <sub>2</sub>	15.0994	C <sub>16</sub> H <sub>34</sub>
8.4536	NH <sub>4</sub> H(C <sub>10</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> ) <sub>2</sub>	15.1721	C <sub>11</sub> H <sub>23</sub> C <sub>6</sub> NH <sub>2</sub>
8.5347	RbH(C <sub>10</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> ) <sub>2</sub>	15.6186	H <sub>2</sub> CC(C <sub>6</sub> H <sub>2</sub> ) <sub>6</sub> CH-(CH <sub>2</sub> ) <sub>7</sub> CH <sub>3</sub>
8.6336	KH(C <sub>10</sub> C <sub>6</sub> H <sub>4</sub> C <sub>6</sub> ) <sub>2</sub>	17.2157	C <sub>19</sub> H <sub>36</sub>
8.9078	C <sub>5</sub> H <sub>11</sub> C <sub>6</sub> NH <sub>2</sub>		

2 2 2

P222 D<sub>2</sub><sup>1</sup> No. 16Inorganic - 4  
Organic - 2

## Inorganic

0.5548	CaU(P <sub>4</sub> ) <sub>2</sub> •1.5H <sub>2</sub> O	0.8742	(U <sub>6</sub> ) <sub>2</sub> V <sub>6</sub> O <sub>17</sub>
0.5603	CaU(P <sub>4</sub> ) <sub>2</sub> •1-2H <sub>2</sub> O	0.9589	H <sub>2</sub> Se <sub>4</sub>

## Organic

0.6667	C <sub>6</sub> H <sub>7</sub> O <sub>5</sub> (CH <sub>3</sub> ) <sub>3</sub>	0.8197	C <sub>6</sub> NH <sub>2</sub> •CH <sub>6</sub> H•CH <sub>6</sub> H•C <sub>6</sub> NH <sub>2</sub>
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2 2 2

P222<sub>1</sub> D<sub>2</sub><sup>2</sup> No. 17Inorganic - 12  
Organic - 15

## Inorganic

0.3588	NaNb <sub>3</sub>	0.7556	Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub>
0.5308	W <sub>6</sub> •Ta <sub>2</sub> O <sub>5</sub>	0.8875	Na <sub>2</sub> CN <sub>2</sub>
0.5472	CsMgF <sub>3</sub>	0.9159	Zr <sub>2</sub> (Cl <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> O
0.5750	KAlSi <sub>4</sub>	0.9528	HfF <sub>4</sub> •H <sub>2</sub> O
0.6512	KH <sub>2</sub> P <sub>5</sub>	0.9621	La <sub>2</sub> (C <sub>6</sub> ) <sub>3</sub> •8H <sub>2</sub> O
0.6957	CF <sub>2</sub> Mo	0.9634	HfF <sub>4</sub> •3H <sub>2</sub> O

## Organic

0.4250	(C <sub>6</sub> H <sub>5</sub> -CH <sub>2</sub> -CH <sub>2</sub> -C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> BK•H <sub>2</sub> O	0.7147	Ta(C <sub>2</sub> H <sub>5</sub> )(C <sub>4</sub> H <sub>9</sub> ) <sub>4</sub>
0.4549	C <sub>21</sub> H <sub>32</sub> O <sub>3</sub>	0.8161	C <sub>20</sub> H <sub>26</sub> O <sub>3</sub>
0.5405	C <sub>6</sub> H <sub>10</sub> O <sub>6</sub>	0.8207	(C <sub>6</sub> H <sub>6</sub> O <sub>6</sub> ) <sub>p</sub> •xH <sub>2</sub> O
0.5480	C <sub>28</sub> H <sub>39</sub> N <sub>5</sub> O <sub>8</sub>	0.8665	C <sub>10</sub> H <sub>7</sub> Cl <sub>2</sub>
0.6164	C <sub>6</sub> H <sub>5</sub> O <sub>8</sub>	0.8875	Na <sub>2</sub> CN <sub>2</sub>
0.6471	C <sub>4</sub> H <sub>5</sub> O <sub>5</sub> NH <sub>2</sub>	0.9028	HgI <sub>2</sub> •C <sub>3</sub> H <sub>6</sub> S <sub>3</sub>
0.6512	C <sub>28</sub> H <sub>34</sub> N <sub>3</sub> O <sub>5</sub> Br	0.9621	La <sub>2</sub> (C <sub>6</sub> ) <sub>3</sub> •8H <sub>2</sub> O
0.6957	Fe <sub>2</sub> MoC		

2 2 2

P2<sub>1</sub>2<sub>1</sub>2 D<sub>2</sub><sup>3</sup> No. 18Inorganic - 24  
Organic - 104

## Inorganic

0.3345	Nb <sub>16</sub> W <sub>18</sub> O <sub>94</sub>	0.6875	Th(Cl <sub>4</sub> ) <sub>4</sub> •4H <sub>2</sub> O
0.3381	Ta <sub>16</sub> W <sub>18</sub> O <sub>94</sub>	0.7555	(RE) <sub>2</sub> (C <sub>6</sub> ) <sub>3</sub> •4H <sub>2</sub> O
0.5137	Cu <sub>3</sub> Se <sub>2</sub>	0.8033	Na <sub>2</sub> HP <sub>4</sub> •2H <sub>2</sub> O
0.5198	NH <sub>4</sub> H <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub>	0.8263	BaS <sub>4</sub> •H <sub>2</sub> O
0.5810	P <sub>4</sub> N <sub>4</sub> (OH) <sub>6</sub> (OK) <sub>2</sub>	0.8305	(Mg, Mn)H <sub>2</sub> O <sub>3</sub>
0.5873	P <sub>4</sub> N <sub>4</sub> (OH) <sub>6</sub> (ORb) <sub>2</sub>	0.8520	K <sub>2</sub> Zn(NCS) <sub>4</sub> •4H <sub>2</sub> O
0.5932	Ca <sub>2</sub> Sn <sub>4</sub>	0.8559	K <sub>2</sub> Co(NCS) <sub>4</sub> •4H <sub>2</sub> O
0.5951	(NH) <sub>4</sub> P <sub>4</sub> O <sub>8</sub> H <sub>4</sub> •2H <sub>2</sub> O	0.8631	BaS <sub>3</sub>
0.5983	Ca <sub>2</sub> Pb <sub>4</sub>	0.9046	CaNi(CN) <sub>4</sub> •5H <sub>2</sub> O
0.5991	P <sub>4</sub> N <sub>4</sub> (OH) <sub>8</sub> •2H <sub>2</sub> O	0.9074	Mo <sub>2</sub> O <sub>8</sub>
0.6118	Sr <sub>2</sub> Pb <sub>4</sub>	0.9244	Na <sub>2</sub> H <sub>2</sub> O <sub>2</sub> •5H <sub>2</sub> O
0.6647	H <sub>3</sub> P <sub>2</sub>	0.9556	CaAl <sub>2</sub> Si <sub>2</sub> O <sub>8</sub>

## Organic

0.3081	[C <sub>19</sub> H <sub>28</sub> Br <sub>2</sub> OH-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> ]	0.3949	C <sub>19</sub> H <sub>26</sub> O <sub>2</sub>
0.3301	C <sub>15</sub> H <sub>26</sub> O	0.4055	C <sub>9</sub> H <sub>14</sub> N <sub>3</sub> O <sub>8</sub> P
0.3581	[C <sub>19</sub> H <sub>31</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> ]	0.4190	[H <sub>2</sub> CC(C <sub>6</sub> H <sub>2</sub> ) <sub>6</sub> CH <sub>2</sub> S] <sub>2</sub> •2HBr
0.3785	[C <sub>28</sub> H <sub>43</sub> OH]	0.4193	C <sub>11</sub> H <sub>17</sub> ON•HI

P<sub>2</sub>1<sub>2</sub>2<sup>2</sup> D<sub>2</sub><sup>3</sup> No. 18 (continued)

## Organic (continued)

0.4275	C <sub>9</sub> H <sub>17</sub> NH <sub>3</sub> I	0.6565	(CH <sub>3</sub> ) <sub>2</sub> -CH-CH <sub>2</sub> -CH(NH <sub>2</sub> )-C <sub>6</sub> H <sub>5</sub>
0.4330	Br•C <sub>6</sub> H <sub>4</sub> •NCS	0.6598	C <sub>19</sub> H <sub>26</sub> Cl <sub>2</sub>
0.4475	Cd[SC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> (HC <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.6867	AgBF <sub>4</sub> •C <sub>3</sub> H <sub>6</sub> S <sub>3</sub> •H <sub>2</sub> O
0.4608	C <sub>21</sub> H <sub>29</sub> N <sub>3</sub> Cl <sub>6</sub>	0.7067	Cd(N <sub>2</sub> H <sub>3</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
0.4642	C <sub>21</sub> H <sub>26</sub> Cl <sub>3</sub> N <sub>2</sub> •HCl	0.7131	(CH <sub>3</sub> •CH•CH) <sub>2</sub> CH <sub>2</sub> N•NH•C <sub>6</sub> H <sub>5</sub> (N <sub>2</sub> ) <sub>2</sub>
0.4667	C <sub>20</sub> H <sub>32</sub> Cl <sub>2</sub>	0.7142	CH <sub>3</sub> N <sub>5</sub> N <sub>2</sub> H <sub>4</sub>
0.4668	C <sub>19</sub> H <sub>23</sub> BrCl <sub>10</sub> S	0.7333	C <sub>10</sub> H <sub>19</sub> NH <sub>2</sub> •HCl
0.4783	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> Cl <sub>4</sub> •C <sub>9</sub> H <sub>11</sub> BrN <sub>2</sub> Cl <sub>6</sub> •H <sub>2</sub> O	0.7368	C <sub>10</sub> H <sub>19</sub> NH <sub>2</sub> •HBr
0.4867	(CH <sub>3</sub> ) <sub>2</sub> C:N•NH•C <sub>6</sub> H <sub>5</sub> (N <sub>2</sub> ) <sub>2</sub>	0.7459	C <sub>10</sub> H <sub>15</sub> ClN•HI
0.4962	C <sub>6</sub> H <sub>13</sub> Cl <sub>5</sub> N•HCl	0.7536	C <sub>2</sub> H <sub>4</sub>
0.4975	C <sub>24</sub> H <sub>40</sub> Cl <sub>4</sub>	0.7555	2(C <sub>6</sub> H <sub>10</sub> Cl <sub>5</sub> ) <sub>6</sub> •3.08(CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> Cl) <sub>4</sub> •19.4H <sub>2</sub> O
0.4980	C <sub>14</sub> H <sub>25</sub> N <sub>3</sub> Cl <sub>9</sub> •HBr•H <sub>2</sub> O	0.7565	(RE) <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> •4H <sub>2</sub> O
0.4988	C <sub>29</sub> H <sub>46</sub> Cl <sub>4</sub>	0.7714	C <sub>6</sub> H <sub>4</sub> (C <sub>6</sub> H <sub>5</sub> )(C <sub>6</sub> H <sub>4</sub> Rb)
0.5133	C <sub>24</sub> H <sub>4</sub> Br <sub>2</sub> •2(C <sub>24</sub> H <sub>40</sub> Cl <sub>4</sub> )	0.7793	(NH <sub>4</sub> ) <sub>2</sub> C <sub>2</sub> Cl <sub>4</sub> •H <sub>2</sub> O
0.5169	C <sub>18</sub> H <sub>32</sub> Cl <sub>16</sub>	0.7794	(NH <sub>4</sub> ) <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •H <sub>2</sub> O
0.5189	C <sub>16</sub> H <sub>32</sub> Cl <sub>2</sub> •8C <sub>24</sub> H <sub>40</sub> Cl <sub>4</sub>	0.8071	C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>
0.5206	C <sub>20</sub> H <sub>30</sub> Cl <sub>2</sub>	0.8076	C <sub>10</sub> H <sub>12</sub> N <sub>5</sub> Cl <sub>4</sub> •C <sub>9</sub> H <sub>12</sub> BrN <sub>3</sub> Cl <sub>4</sub>
0.5224	C <sub>18</sub> H <sub>36</sub> Cl <sub>2</sub> •8C <sub>24</sub> H <sub>40</sub> Cl <sub>4</sub>	0.8187	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub> •HBr
0.5229	C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> •4C <sub>24</sub> H <sub>40</sub> Cl <sub>4</sub>	0.8262	C <sub>14</sub> H <sub>20</sub> Cl <sub>4</sub> N <sub>2</sub> S•1.5H <sub>2</sub> O
0.5231	C <sub>12</sub> H <sub>24</sub> Cl <sub>2</sub> •6C <sub>24</sub> H <sub>40</sub> Cl <sub>4</sub>	0.8343	KNaC <sub>4</sub> H <sub>4</sub> Cl <sub>6</sub> •4H <sub>2</sub> O
0.5232	2(C <sub>24</sub> H <sub>40</sub> Cl <sub>4</sub> )•C <sub>3</sub> H <sub>6</sub> Cl <sub>6</sub>	0.8368	C <sub>4</sub> H <sub>4</sub> Cl <sub>6</sub> RbNa•4H <sub>2</sub> O
0.5239	C <sub>8</sub> H <sub>16</sub> Cl <sub>2</sub> •4C <sub>24</sub> H <sub>40</sub> Cl <sub>4</sub>	0.8419	C <sub>6</sub> H <sub>4</sub> (C <sub>6</sub> H <sub>5</sub> )(C <sub>6</sub> H <sub>4</sub> Ca)
0.5246	C <sub>7</sub> H <sub>14</sub> Cl <sub>2</sub> •4C <sub>24</sub> H <sub>40</sub> Cl <sub>4</sub>	0.8457	Zr(C <sub>4</sub> H <sub>3</sub> S•C <sub>6</sub> H <sub>5</sub> •C <sub>6</sub> H <sub>4</sub> •CF <sub>3</sub> ) <sub>4</sub>
0.5262	C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> •3C <sub>24</sub> H <sub>40</sub> Cl <sub>4</sub>	0.8460	Pu(C <sub>4</sub> H <sub>3</sub> S•C <sub>6</sub> H <sub>5</sub> •C <sub>6</sub> H <sub>4</sub> •CF <sub>3</sub> ) <sub>4</sub>
0.5273	C <sub>18</sub> H <sub>24</sub> Cl <sub>2</sub> •C <sub>2</sub> H <sub>6</sub> Cl <sub>6</sub>	0.8462	Ce(C <sub>4</sub> H <sub>3</sub> S•C <sub>6</sub> H <sub>5</sub> •C <sub>6</sub> H <sub>4</sub> •CF <sub>3</sub> ) <sub>4</sub>
0.5315	C <sub>6</sub> H <sub>12</sub> Cl <sub>5</sub>	0.8463	Hf(C <sub>4</sub> H <sub>3</sub> S•C <sub>6</sub> H <sub>5</sub> •C <sub>6</sub> H <sub>4</sub> •CF <sub>3</sub> ) <sub>4</sub>
0.5366	C <sub>24</sub> H <sub>42</sub> Cl <sub>2</sub> •4H <sub>2</sub> O	0.8520	K <sub>2</sub> Zn(NCS) <sub>4</sub> •4H <sub>2</sub> O
0.5374	CH <sub>2</sub> Cl(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> CH <sub>2</sub> Cl	0.8559	K <sub>2</sub> Co(NCS) <sub>4</sub> •4H <sub>2</sub> O
0.5380	NH <sub>4</sub> Li•C <sub>4</sub> H <sub>4</sub> Cl <sub>6</sub> •H <sub>2</sub> O	0.8649	Th(C <sub>4</sub> H <sub>3</sub> S•C <sub>6</sub> H <sub>5</sub> •C <sub>6</sub> H <sub>4</sub> •CF <sub>3</sub> ) <sub>4</sub>
0.5386	LiRbC <sub>4</sub> H <sub>4</sub> Cl <sub>6</sub> •H <sub>2</sub> O	0.8789	C <sub>22</sub> H <sub>34</sub> BrN <sub>5</sub> Cl•0.5CH <sub>3</sub> Cl
0.5386	LiTlC <sub>4</sub> H <sub>4</sub> Cl <sub>6</sub> •H <sub>2</sub> O	0.8869	C <sub>19</sub> H <sub>27</sub> Cl <sub>7</sub> •C <sub>6</sub> H <sub>5</sub> •CH <sub>3</sub>
0.5475	KLiC <sub>4</sub> H <sub>4</sub> Cl <sub>6</sub> •H <sub>2</sub> O	0.8982	NH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> NH <sub>3</sub> •S <sub>7</sub>
0.5535	C <sub>16</sub> H <sub>14</sub> Cl <sub>3</sub>	0.9046	CaNi(CN) <sub>4</sub> •5H <sub>2</sub> O
0.5567	C <sub>28</sub> H <sub>39</sub> N <sub>5</sub> Cl <sub>8</sub>	0.9125	HgBr <sub>2</sub> •C <sub>3</sub> H <sub>6</sub> S <sub>3</sub>
0.5571	C <sub>22</sub> H <sub>25</sub> N <sub>5</sub> Cl <sub>6</sub> •HAuCl <sub>4</sub>	0.9168	C <sub>10</sub> H <sub>20</sub> Cl <sub>6</sub>
0.5652	Fe <sub>3</sub> (CH <sub>3</sub> COCl) <sub>6</sub> Cl•5H <sub>2</sub> O	0.9285	[Co(CH <sub>3</sub> ) <sub>3</sub> ] <sub>2</sub> •C <sub>4</sub> H <sub>2</sub> •S <sub>2</sub>
0.5703	C <sub>19</sub> H <sub>23</sub> N <sub>3</sub> Cl <sub>3</sub>	0.9421	C <sub>7</sub> H <sub>13</sub> BrCl <sub>5</sub>
0.5770	(NH <sub>4</sub> ) <sub>2</sub> (VO) <sub>2</sub> (C <sub>2</sub> Cl <sub>4</sub> ) <sub>3</sub> •6H <sub>2</sub> O	0.9461	C <sub>24</sub> H <sub>28</sub> Br <sub>2</sub> Cl <sub>8</sub>
0.5819	C <sub>6</sub> H <sub>9</sub> Cl <sub>6</sub> (CH <sub>3</sub> ) <sub>3</sub>	0.9483	Co <sub>2</sub> (CNCH <sub>3</sub> ) <sub>10</sub> (Cl <sub>4</sub> ) <sub>4</sub>
0.5905	Cr <sub>3</sub> (CH <sub>3</sub> COCl) <sub>6</sub> Cl•5H <sub>2</sub> O	0.9525	(CH <sub>2</sub> ) <sub>4</sub> (NH <sub>3</sub> ) <sub>2</sub> S <sub>6</sub>
0.5918	(CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> SeBr <sub>2</sub>	0.9688	C <sub>20</sub> H <sub>25</sub> N <sub>4</sub> N <sub>3</sub> Cl <sub>15</sub> P <sub>2</sub> •12H <sub>2</sub> O
0.5937	C <sub>14</sub> H <sub>14</sub> SeCl <sub>2</sub>	0.9765	C <sub>10</sub> H <sub>18</sub> N <sub>4</sub> NiCl <sub>4</sub>
0.6017	C <sub>20</sub> H <sub>24</sub> Cl <sub>2</sub> N <sub>2</sub> •2HBr•3H <sub>2</sub> O	0.9812	C <sub>21</sub> H <sub>27</sub> N <sub>5</sub> HCl•H <sub>2</sub> O
0.6067	C <sub>25</sub> H <sub>23</sub> I <sub>8</sub>	0.9821	C <sub>6</sub> H <sub>8</sub> Cl <sub>2</sub> Br <sub>2</sub>
0.6127	CH <sub>3</sub> •CH•N•NH•C <sub>6</sub> H <sub>5</sub> (N <sub>2</sub> ) <sub>2</sub>	0.9841	C <sub>6</sub> H <sub>8</sub> Cl <sub>4</sub>
0.6251	C <sub>18</sub> H <sub>24</sub> Cl <sub>2</sub>	0.9877	(CH <sub>3</sub> ) <sub>2</sub> C:N•C <sub>6</sub> H <sub>5</sub> •Cl
0.6304	(CH <sub>2</sub> ) <sub>3</sub> (NH <sub>3</sub> ) <sub>2</sub> S <sub>5</sub>	0.9900	C <sub>6</sub> H <sub>8</sub> Br <sub>4</sub>
0.6413	C <sub>21</sub> H <sub>29</sub> BrN <sub>2</sub> Cl <sub>4</sub> •4H <sub>2</sub> O	0.9943	C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> Cl <sub>9</sub> (CH <sub>2</sub> ) <sub>4</sub> Cl <sub>2</sub>

2 2 2

P<sub>2</sub>1<sub>2</sub>2<sup>1</sup> D<sub>2</sub><sup>4</sup> No. 19Inorganic - 88  
Organic - 722

## Inorganic

0.3976	Tl <sub>2</sub> S <sub>5</sub>	0.6480	HN <sub>3</sub> •3H <sub>2</sub> O
0.4003	PbAs <sub>2</sub> S <sub>4</sub>	0.6557	H <sub>2</sub> SeCl <sub>3</sub>
0.4107	K[Au(CN) <sub>4</sub> ] <sub>2</sub> •H <sub>2</sub> O	0.6563	Be(CH <sub>3</sub> ) <sub>2</sub>
0.4223	Tl <sub>2</sub> Sn <sub>3</sub>	0.6666	SnF <sub>2</sub>
0.4278	PbAs <sub>2</sub> S <sub>4</sub>	0.6685	H <sub>2</sub> N <sub>2</sub> H
0.4281	Rb <sub>2</sub> Sn <sub>3</sub>	0.6859	Ce <sub>2</sub> Sn <sub>4</sub> •H <sub>2</sub> O
0.4328	NH <sub>4</sub> Sn <sub>3</sub>	0.7057	CaSn <sub>3</sub>
0.4334	Zn <sub>2</sub> (OH) <sub>2</sub> S <sub>4</sub>	0.7277	U <sub>6</sub>
0.4398	Cu <sub>2</sub> (OH) <sub>3</sub> (N <sub>3</sub> )	0.7353	N <sub>2</sub> H <sub>5</sub> H <sub>2</sub> P <sub>4</sub>
0.4451	BaGe <sub>3</sub>	0.7398	Cd(BrCl <sub>3</sub> ) <sub>2</sub> •2H <sub>2</sub> O
0.5148	Hg(Cl, Br) <sub>2</sub>	0.7410	(Ca, Na) <sub>2</sub> ReSi <sub>2</sub> (Cl, OH, F) <sub>7</sub>
0.5760	NH <sub>4</sub> OH	0.7430	Bi <sub>2</sub> Cu <sub>6</sub> S <sub>6</sub>
0.5874	K <sub>2</sub> SO <sub>3</sub> NH <sub>2</sub>	0.7589	HI <sub>3</sub>
0.6049	Zn(OH) <sub>2</sub>	0.7595	Xe <sub>3</sub>
0.6229	GeF <sub>2</sub>	0.7683	KH <sub>2</sub> F <sub>3</sub>
0.6268	Cu <sub>3</sub> Mo <sub>2</sub> Cl <sub>8</sub>	0.7731	CuTe <sub>3</sub> •2H <sub>2</sub> O
0.6390	NaNH <sub>4</sub> SO <sub>4</sub> •2H <sub>2</sub> O	0.7962	(NPCL <sub>2</sub> ) <sub>5</sub>
0.6400	MgCO <sub>3</sub> •3H <sub>2</sub> O	0.7966	Pb <sub>3</sub> Cl <sub>2</sub>

P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub> D<sub>2</sub><sup>4</sup> No. 19 (continued)

## Inorganic (continued)

0.7983	Pb <sub>3</sub> Cl <sub>2</sub>	0.9008	Pb <sub>8</sub> Bi <sub>6</sub> S <sub>17</sub>
0.8032	CuSe <sub>3</sub> •2H <sub>2</sub> O	0.9009	N <sub>2</sub> H <sub>6</sub> S <sub>6</sub>
0.8035	CaCu(OH)As <sub>2</sub> O <sub>4</sub>	0.9128	K <sub>2</sub> [B <sub>4</sub> O <sub>5</sub> (OH) <sub>4</sub> ]•2H <sub>2</sub> O
0.8052	CaCu(OH)(VO <sub>4</sub> )	0.9447	AlB <sub>12</sub>
0.8088	CuSe <sub>3</sub> •2H <sub>2</sub> O	0.9450	BaSnSe <sub>3</sub>
0.8095	CuPb(OH)(VO <sub>4</sub> )	0.9465	B <sub>8</sub> Cl <sub>8</sub>
0.8221	Re <sub>2</sub> O <sub>7</sub>	0.9536	Ba <sub>2</sub> Bi <sub>2</sub> Se <sub>5</sub>
0.8222	CuHP <sub>3</sub> •2H <sub>2</sub> O	0.9556	Cu <sub>2</sub> (OH)As <sub>2</sub> O <sub>4</sub>
0.8228	SbBr <sub>3</sub>	0.9572	Cu <sub>2</sub> (OH)As <sub>2</sub> O <sub>4</sub> •3H <sub>2</sub> O
0.8255	CaZn(OH)As <sub>2</sub> O <sub>4</sub>	0.9575	NaAlCl <sub>4</sub>
0.8356	CaMgOHAs <sub>2</sub> O <sub>4</sub>	0.9589	NaFeCl <sub>4</sub>
0.8393	AsBr <sub>3</sub>	0.9712	NH <sub>4</sub> Br•3NH <sub>3</sub>
0.8409	AsBr <sub>3</sub>	0.9769	HgCl <sub>2</sub> SCN
0.8433	AsBr <sub>3</sub>	0.9784	NH <sub>4</sub> Cl•3NH <sub>3</sub>
0.8519	[(NH <sub>3</sub> ) <sub>5</sub> Co <sub>2</sub> ](HSO <sub>4</sub> ) <sub>3</sub> SO <sub>4</sub> •3H <sub>2</sub> O	0.9801	ZnSO <sub>4</sub> •7H <sub>2</sub> O
0.8524	(NH <sub>3</sub> ) <sub>5</sub> Co <sub>2</sub> Co(NH <sub>3</sub> ) <sub>5</sub> (SO <sub>4</sub> )(HSO <sub>4</sub> ) <sub>3</sub>	0.9815	NiSO <sub>4</sub> •7H <sub>2</sub> O
0.8548	Li <sub>2</sub> ZnCl <sub>4</sub> •2H <sub>2</sub> O	0.9871	(Ni, Mg)SO <sub>4</sub> •7H <sub>2</sub> O
0.8630	Hg(OH)F	0.9893	MgSO <sub>4</sub> •7H <sub>2</sub> O
0.8666	Co(NH <sub>3</sub> ) <sub>3</sub> (NO <sub>2</sub> ) <sub>3</sub>	0.9901	MgCr <sub>2</sub> O <sub>4</sub> •7H <sub>2</sub> O
0.8725	Al <sub>6</sub> (OH) <sub>6</sub> (PO <sub>4</sub> ) <sub>4</sub> •5H <sub>2</sub> O	0.9925	MgSO <sub>4</sub> •7H <sub>2</sub> O
0.8782	NH <sub>4</sub> [Co(NH <sub>3</sub> ) <sub>2</sub> (NO <sub>2</sub> ) <sub>4</sub> ]	0.9934	NH <sub>4</sub> D <sub>2</sub> PO <sub>4</sub>
0.8784	Tl <sub>2</sub> SO <sub>4</sub> •H <sub>2</sub> O	0.9973	NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub>
0.8788	K[Co(NH <sub>3</sub> ) <sub>2</sub> (NO <sub>2</sub> ) <sub>4</sub> ]	1.0000	Rb <sub>2</sub> Ge <sub>8</sub> O <sub>17</sub>
0.8803	Ca <sub>2</sub> (OH)(Si <sub>2</sub> O <sub>7</sub> )	1.0000	K <sub>2</sub> Ge <sub>8</sub> O <sub>17</sub>
0.8832	K[Co(NH <sub>3</sub> ) <sub>2</sub> (NO <sub>2</sub> ) <sub>4</sub> ]	1.0000	MoNi
0.8847	NH <sub>4</sub> [Co(NO <sub>2</sub> ) <sub>4</sub> (NH <sub>3</sub> ) <sub>2</sub> ]	1.0000	Si <sub>2</sub>

## Organic

0.0785	C <sub>18</sub> H <sub>37</sub> NH <sub>3</sub> Cl	0.2732	C <sub>27</sub> H <sub>39</sub> O <sub>3</sub> N•HCl•CH <sub>3</sub> OH
0.0893	C <sub>21</sub> H <sub>42</sub> O <sub>4</sub>	0.2790	C <sub>27</sub> H <sub>44</sub> O <sub>6</sub>
0.1202	[CH <sub>3</sub> (CH <sub>2</sub> ) <sub>10</sub> COO]C <sub>3</sub> H <sub>7</sub> O <sub>2</sub>	0.2806	Cl•C <sub>6</sub> H <sub>4</sub> •CH•N•OH
0.1387	[C <sub>19</sub> H <sub>28</sub> OH-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH(C <sub>2</sub> H <sub>5</sub> )CH(CH <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> O]	0.2808	C <sub>10</sub> H <sub>15</sub> OH•HBr
0.1589	NO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> •CO•O-C <sub>19</sub> H <sub>28</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH(C <sub>2</sub> H <sub>5</sub> )CH(CH <sub>3</sub> ) <sub>2</sub>	0.2810	C <sub>10</sub> H <sub>6</sub> O <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub>
0.1628	C <sub>25</sub> H <sub>40</sub> O <sub>4</sub>	0.2824	C <sub>32</sub> H <sub>53</sub> O <sub>2</sub> I
0.1833	C <sub>6</sub> H <sub>5</sub> •CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> •HCl	0.2869	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub> •HBr•H <sub>2</sub> O
0.1886	[C <sub>19</sub> H <sub>28</sub> Br <sub>2</sub> Cl-CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> ]	0.2893	C <sub>12</sub> H <sub>6</sub> O <sub>2</sub>
0.1901	[CH <sub>3</sub> CH <sub>2</sub> OC <sub>19</sub> H <sub>28</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> ]	0.2947	C <sub>22</sub> H <sub>28</sub> O <sub>4</sub>
0.1906	C <sub>18</sub> H <sub>34</sub> O <sub>4</sub>	0.2967	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub> •HBr
0.1924	C <sub>6</sub> H <sub>5</sub> •CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> •HBr	0.3048	(C <sub>10</sub> H <sub>6</sub> ) <sub>2</sub> •C <sub>6</sub> H <sub>3</sub> (NO <sub>2</sub> ) <sub>3</sub>
0.1929	C <sub>27</sub> H <sub>42</sub> O <sub>5</sub>	0.3055	C <sub>13</sub> H <sub>12</sub> O <sub>2</sub> •C <sub>11</sub> H <sub>10</sub> O <sub>2</sub> S
0.1930	CH <sub>3</sub> •CO•OC <sub>19</sub> H <sub>28</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>	0.3066	(CH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> O
0.1952	C <sub>20</sub> H <sub>25</sub> N <sub>3</sub> O <sub>6</sub> •HBr	0.3084	C <sub>16</sub> H <sub>17</sub> O <sub>4</sub> N <sub>2</sub> SK
0.2097	C <sub>12</sub> H <sub>17</sub> BrN <sub>2</sub> O <sub>5</sub>	0.3116	[C <sub>19</sub> H <sub>29</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub> ]
0.2167	[CH <sub>3</sub> •CO•O-C <sub>19</sub> H <sub>28</sub> -CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub> ]	0.3129	C <sub>16</sub> H <sub>17</sub> N <sub>2</sub> O <sub>4</sub> SRb
0.2238	(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> N=C•NC <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	0.3138	C <sub>10</sub> H <sub>17</sub> N <sub>3</sub> O <sub>6</sub> S
0.2252	[C <sub>18</sub> H <sub>22</sub> OH-CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub> ]	0.3141	CH <sub>2</sub> OH(CH <sub>2</sub> ) <sub>4</sub> CO <sub>2</sub> Rb
0.2286	C <sub>23</sub> H <sub>26</sub> IN <sub>4</sub> •CH <sub>3</sub> OH	0.3148	[(CO) <sub>9</sub> Co <sub>3</sub> ]CCOC[Co <sub>3</sub> (CO) <sub>9</sub> ]
0.2300	C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub> •HBr	0.3154	C <sub>14</sub> H <sub>16</sub> N <sub>2</sub>
0.2319	C <sub>21</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub> •HBr•2H <sub>2</sub> O	0.3156	SO <sub>2</sub> (C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> ) <sub>2</sub>
0.2343	[OC <sub>6</sub> H <sub>7</sub> (CO•CH <sub>3</sub> ) <sub>4</sub> -OC <sub>19</sub> H <sub>28</sub> -CH(CH <sub>3</sub> )CH=CHCH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub> ]	0.3157	CH <sub>2</sub> OH(CH <sub>2</sub> ) <sub>4</sub> CO <sub>2</sub> K
0.2350	C <sub>9</sub> H <sub>9</sub> Cl <sub>3</sub> O <sub>3</sub>	0.3159	(CH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> S
0.2367	C <sub>28</sub> H <sub>46</sub> Br <sub>2</sub>	0.3159	C <sub>30</sub> H <sub>46</sub> N <sub>6</sub> O <sub>5</sub> •HI•xH <sub>2</sub> O
0.2401	(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> OH	0.3178	(CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> Te
0.2522	C <sub>6</sub> H <sub>5</sub> •CH <sub>2</sub> •CH(NH <sub>2</sub> )COOH•HCl	0.3181	(CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> Se
0.2545	C <sub>27</sub> H <sub>43</sub> O <sub>5</sub> •CO•C <sub>6</sub> H <sub>4</sub> Br	0.3191	C <sub>23</sub> H <sub>30</sub> O <sub>6</sub> •2H <sub>2</sub> O
0.2564	C <sub>23</sub> H <sub>25</sub> BrO <sub>5</sub>	0.3194	C <sub>15</sub> H <sub>17</sub> BrO <sub>6</sub>
0.2600	C <sub>10</sub> H <sub>15</sub> N(CH <sub>3</sub> ) <sub>3</sub> I	0.3196	C <sub>37</sub> H <sub>54</sub> O <sub>2</sub>
0.2608	(CH <sub>3</sub> ZnOCH <sub>3</sub> ) <sub>4</sub>	0.3204	CO(O <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
0.2637	C <sub>10</sub> H <sub>15</sub> OH•C <sub>4</sub> H <sub>6</sub> O <sub>6</sub> •H <sub>2</sub> O	0.3216	C <sub>16</sub> H <sub>15</sub> NaN <sub>2</sub> O <sub>6</sub> S <sub>2</sub>
0.2661	BrC <sub>6</sub> H <sub>4</sub> CO•CH	0.3223	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> •HCl•H <sub>2</sub> O
0.2662	C <sub>18</sub> H <sub>13</sub> As	0.3251	C <sub>20</sub> H <sub>21</sub> NO <sub>4</sub>
0.2665	C <sub>10</sub> H <sub>15</sub> O <sub>4</sub> N	0.3260	C <sub>32</sub> H <sub>54</sub> O <sub>2</sub>
0.2666	C <sub>8</sub> H <sub>15</sub> NO <sub>2</sub> •HBr	0.3268	[C <sub>19</sub> H <sub>29</sub> Br <sub>2</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> ]
0.2680	(C <sub>2</sub> H <sub>5</sub> )(C <sub>6</sub> H <sub>5</sub> )C <sub>5</sub> H <sub>5</sub> NO <sub>2</sub>	0.3335	C <sub>19</sub> H <sub>28</sub> O <sub>2</sub>
0.2686	C <sub>9</sub> H <sub>17</sub> NO <sub>2</sub> •HBr	0.3347	C <sub>10</sub> H <sub>4</sub> (NO <sub>2</sub> ) <sub>4</sub>
0.2711	C <sub>10</sub> H <sub>15</sub> OH•HCl	0.3357	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>
0.2714	C <sub>12</sub> H <sub>6</sub> O <sub>2</sub>	0.3358	C <sub>13</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub> •H <sub>2</sub> O
0.2715	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub> HCl•H <sub>2</sub> O	0.3409	C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub> •HCl
0.2728	C <sub>37</sub> H <sub>52</sub> O <sub>2</sub>	0.3411	[C <sub>19</sub> H <sub>27</sub> (OH) <sub>2</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> ]
0.2728	C <sub>37</sub> H <sub>56</sub> O <sub>2</sub>	0.3413	C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub> •HI
0.2730	C <sub>27</sub> H <sub>39</sub> O <sub>3</sub> N•HBr•CH <sub>3</sub> OH	0.3419	C <sub>48</sub> H <sub>40</sub> I <sub>2</sub> O <sub>16</sub>
		0.3425	C <sub>19</sub> H <sub>31</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>
		0.3426	(C <sub>6</sub> H <sub>5</sub> S) <sub>2</sub>

P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub> D<sub>2</sub><sup>4</sup> No. 19 (continued)

## Organic (continued)

0.3436	C <sub>12</sub> H <sub>10</sub> Se <sub>2</sub>	0.4357	NH <sub>4</sub> CoC <sub>2</sub> H <sub>4</sub> N <sub>2</sub> (CH <sub>2</sub> Cθθ) <sub>4</sub> •2H <sub>2</sub> θ
0.3436	C <sub>20</sub> H <sub>12</sub>	0.4361	C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> θ <sub>4</sub> •4H <sub>2</sub> θ
0.3462	(C <sub>5</sub> H <sub>5</sub> )Fe(C <sub>5</sub> H <sub>4</sub> •Cθθ•C <sub>6</sub> H <sub>3</sub> [θCH <sub>3</sub> ] <sub>2</sub> )	0.4371	RbCr(C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> θ <sub>8</sub> )•2H <sub>2</sub> θ
0.3491	C <sub>19</sub> H <sub>24</sub> θ <sub>3</sub>	0.4373	C <sub>9</sub> H <sub>15</sub> θ <sub>6</sub>
0.3493	C <sub>7</sub> H <sub>14</sub> θ <sub>6</sub> •H <sub>2</sub> θ	0.4382	C <sub>16</sub> H <sub>22</sub> θ <sub>6</sub>
0.3495	C <sub>8</sub> H <sub>20</sub> Pθ <sub>6</sub> N•CdCl <sub>2</sub> •3H <sub>2</sub> θ	0.4386	C <sub>10</sub> H <sub>7</sub> •C <sub>6</sub> H <sub>5</sub> •CH <sub>3</sub> •SiH
0.3547	C <sub>15</sub> H <sub>17</sub> Brθ <sub>3</sub>	0.4411	PbCo(C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> θ <sub>8</sub> )•2H <sub>2</sub> θ
0.3555	C <sub>19</sub> H <sub>31</sub> -CH(CH <sub>3</sub> )Cθ <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	0.4411	C <sub>10</sub> H <sub>7</sub> •C <sub>6</sub> H <sub>5</sub> •CH <sub>3</sub> •SiF
0.3558	C <sub>12</sub> H <sub>14</sub> θ <sub>11</sub> (Cθ•C <sub>3</sub> H <sub>7</sub> ) <sub>8</sub>	0.4412	C <sub>7</sub> H <sub>12</sub> θ <sub>7</sub>
0.3560	C <sub>4</sub> Cl <sub>2</sub> H <sub>8</sub> θ <sub>3</sub>	0.4422	C <sub>13</sub> H <sub>15</sub> Nθ <sub>2</sub> •HBr•H <sub>2</sub> θ
0.3571	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> CH(NH <sub>2</sub> )CθθH	0.4423	C <sub>12</sub> H <sub>22</sub> θ <sub>11</sub> •NaCl•2H <sub>2</sub> θ
0.3615	C <sub>6</sub> H <sub>12</sub> θ <sub>6</sub>	0.4428	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> θ <sub>2</sub> •HBr•0.5H <sub>2</sub> θ
0.3655	HSCH <sub>2</sub> CH(NH <sub>2</sub> )CθθH•HCl•H <sub>2</sub> θ	0.4430	C <sub>18</sub> H <sub>20</sub> θ <sub>6</sub> N <sub>3</sub> S <sub>2</sub> Cl•0.65CH <sub>2</sub> Br <sub>2</sub>
0.3669	[C <sub>19</sub> H <sub>28</sub> (θH) <sub>3</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> ]	0.4434	C <sub>12</sub> H <sub>22</sub> θ <sub>11</sub> •NaBr•2H <sub>2</sub> θ
0.3693	C <sub>32</sub> H <sub>52</sub> θ <sub>2</sub>	0.4449	C <sub>17</sub> H <sub>28</sub> θ <sub>9</sub> NI
0.3701	C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> θ <sub>5</sub> S	0.4450	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>
0.3713	C <sub>19</sub> H <sub>31</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> Cθ <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	0.4451	C <sub>23</sub> H <sub>33</sub> Brθ <sub>3</sub> •C <sub>7</sub> H <sub>16</sub>
0.3730	CH <sub>2</sub> (NH <sub>2</sub> )CθθH•HNO <sub>3</sub>	0.4457	C <sub>15</sub> H <sub>14</sub> Br <sub>2</sub> θ <sub>8</sub>
0.3757	C <sub>15</sub> H <sub>20</sub> θ <sub>4</sub>	0.4457	C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> θ <sub>4</sub> •HBr
0.3762	C <sub>15</sub> H <sub>17</sub> Brθ <sub>6</sub>	0.4460	C <sub>17</sub> H <sub>28</sub> θ <sub>9</sub> NBr
0.3777	C <sub>27</sub> H <sub>44</sub> θ <sub>6</sub> •0.5H <sub>2</sub> θ	0.4478	CH <sub>3</sub> •Sθ•CH <sub>2</sub> •CH(NH <sub>2</sub> )•Cθθ•θH
0.3785	C <sub>12</sub> H <sub>8</sub> θ <sub>8</sub>	0.4491	C <sub>10</sub> H <sub>7</sub> •C <sub>6</sub> H <sub>5</sub> •CH <sub>3</sub> •SiCl
0.3805	C <sub>28</sub> H <sub>36</sub> -38θ <sub>4</sub>	0.4520	2(C <sub>2</sub> H <sub>5</sub> Nθ <sub>2</sub> )•HCl
0.3821	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> Sθ <sub>2</sub> •H <sub>2</sub> θ	0.4567	C <sub>23</sub> H <sub>33</sub> N <sub>2</sub> θ <sub>2</sub> I
0.3829	C <sub>12</sub> H <sub>8</sub> θ <sub>8</sub> Se	0.4595	C <sub>23</sub> H <sub>32</sub> θ <sub>3</sub>
0.3852	C <sub>9</sub> H <sub>15</sub> N <sub>3</sub> θ <sub>6</sub> •H <sub>2</sub> θ	0.4623	C <sub>24</sub> H <sub>33</sub> Brθ <sub>8</sub>
0.3860	C <sub>9</sub> H <sub>6</sub> θ <sub>2</sub>	0.4651	(CH <sub>3</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>9</sub> θ <sub>6</sub>
0.3869	C <sub>12</sub> H <sub>21</sub> N <sub>3</sub> θ <sub>5</sub> •2HCl	0.4662	C <sub>24</sub> H <sub>35</sub> Iθ <sub>4</sub>
0.3869	C <sub>24</sub> H <sub>40</sub> θ <sub>4</sub>	0.4674	C <sub>6</sub> H <sub>12</sub> θ <sub>5</sub>
0.3903	C <sub>16</sub> H <sub>25</sub> Nθ	0.4707	(CH <sub>3</sub> Nθ) <sub>2</sub>
0.3948	C <sub>20</sub> H <sub>12</sub> N <sub>2</sub>	0.4712	C <sub>32</sub> H <sub>52</sub> Br <sub>2</sub> θ <sub>3</sub>
0.3966	BrC <sub>6</sub> H <sub>4</sub> •C <sub>4</sub> H <sub>4</sub> Nθ <sub>2</sub>	0.4724	C <sub>22</sub> H <sub>27</sub> Nθ <sub>7</sub>
0.3980	C <sub>12</sub> H <sub>8</sub> θ <sub>8</sub> Te	0.4725	Ag(NH <sub>2</sub> CSNHNH <sub>2</sub> )Br
0.3987	(C <sub>6</sub> H <sub>10</sub> θ <sub>5</sub> ) <sub>6</sub> I <sub>2</sub> •14H <sub>2</sub> θ	0.4725	NH <sub>2</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>10</sub> CθθH
0.3990	C <sub>11</sub> H <sub>15</sub> BrN <sub>2</sub> θ <sub>4</sub>	0.4740	C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> θ <sub>2</sub> •H <sub>2</sub> θ
0.3996	(CH <sub>3</sub> ) <sub>4</sub> C <sub>6</sub> H <sub>8</sub> θ <sub>6</sub>	0.4753	C <sub>10</sub> H <sub>8</sub> NNaθ <sub>3</sub> S
0.4008	C <sub>3</sub> H <sub>5</sub> (NH <sub>2</sub> )(CθθH) <sub>2</sub>	0.4770	C <sub>10</sub> H <sub>8</sub> KNθ <sub>3</sub> S
0.4012	C <sub>25</sub> H <sub>40</sub> θ <sub>4</sub>	0.4798	AgCl•NH <sub>2</sub> CSNHNH <sub>2</sub>
0.4014	(CH <sub>3</sub> [CH <sub>2</sub> ] <sub>10</sub> Cθθ) <sub>3</sub> C <sub>3</sub> H <sub>5</sub>	0.4798	C <sub>4</sub> H <sub>6</sub> Br <sub>2</sub> θ <sub>2</sub>
0.4020	C <sub>30</sub> H <sub>50</sub> θ <sub>2</sub>	0.4800	C <sub>17</sub> H <sub>21</sub> θ <sub>4</sub> N•HCl
0.4040	C <sub>30</sub> H <sub>41</sub> Iθ <sub>4</sub>	0.4804	LiCl•C <sub>5</sub> H <sub>5</sub> N
0.4051	C <sub>15</sub> H <sub>24</sub> θ <sub>2</sub>	0.4814	C <sub>22</sub> H <sub>35</sub> θ <sub>2</sub> N•HBr•H <sub>2</sub> θ
0.4076	C <sub>7</sub> H <sub>9</sub> N <sub>3</sub> θ <sub>2</sub> •2H <sub>2</sub> θ	0.4847	Hθ <sub>2</sub> C•C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub> CθθH <sub>2</sub>
0.4080	C <sub>21</sub> H <sub>30</sub> θ <sub>5</sub>	0.4859	C <sub>30</sub> H <sub>50</sub> θ
0.4107	K[Au(CN) <sub>4</sub> ] <sub>2</sub> •H <sub>2</sub> θ	0.4887	Zn(C <sub>10</sub> H <sub>7</sub> Sθ <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> θ
0.4118	C <sub>24</sub> H <sub>40</sub> θ <sub>4</sub>	0.4887	C <sub>3</sub> H <sub>7</sub> Nθ <sub>2</sub>
0.4130	C <sub>23</sub> H <sub>30</sub> θ <sub>6</sub>	0.4898	C <sub>10</sub> H <sub>15</sub> BrClNθ
0.4132	C <sub>21</sub> H <sub>22</sub> θ <sub>10</sub>	0.4904	C <sub>35</sub> H <sub>46</sub> INθ <sub>4</sub>
0.4134	C <sub>10</sub> H <sub>13</sub> BrN <sub>2</sub> θ <sub>4</sub>	0.4929	C <sub>10</sub> H <sub>16</sub> θ <sub>3</sub> N <sub>2</sub> S
0.4142	C <sub>22</sub> H <sub>29</sub> BrN <sub>2</sub> θ <sub>4</sub> •2H <sub>2</sub> θ	0.4933	C <sub>17</sub> H <sub>21</sub> Nθ <sub>4</sub> •HBr
0.4160	HθC <sub>19</sub> H <sub>30</sub> •CH(θH)CH <sub>3</sub>	0.4938	C <sub>23</sub> H <sub>32</sub> N <sub>4</sub> θ <sub>7</sub>
0.4162	C <sub>23</sub> H <sub>31</sub> BrN <sub>2</sub> θ <sub>4</sub>	0.4954	(C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> θ <sub>8</sub> ) <sub>2</sub> H <sub>2</sub> Sθ <sub>4</sub> •C <sub>4</sub> H <sub>8</sub> θ <sub>4</sub> •10H <sub>2</sub> θ
0.4191	C <sub>6</sub> H <sub>12</sub> θ <sub>6</sub>	0.4960	CH <sub>3</sub> CH(NH <sub>2</sub> )CθθH
0.4191	C <sub>21</sub> H <sub>30</sub> θ <sub>3</sub>	0.4962	C <sub>32</sub> H <sub>52</sub> θ <sub>2</sub>
0.4206	C <sub>22</sub> H <sub>33</sub> θ <sub>3</sub>	0.4963	C <sub>3</sub> H <sub>7</sub> N <sub>5</sub> •HCl
0.4213	C <sub>16</sub> H <sub>21</sub> Brθ <sub>7</sub>	0.4970	(C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> θ <sub>8</sub> ) <sub>2</sub> H <sub>2</sub> Sθ <sub>4</sub> •C <sub>3</sub> H <sub>4</sub> θ <sub>4</sub> •10H <sub>2</sub> θ
0.4228	C <sub>15</sub> H <sub>24</sub> θ <sub>2</sub>	0.5007	C <sub>28</sub> H <sub>31</sub> Iθ <sub>6</sub>
0.4230	C <sub>25</sub> H <sub>42</sub> θ <sub>3</sub>	0.5011	C <sub>15</sub> H <sub>15</sub> Brθ <sub>6</sub>
0.4230	C <sub>17</sub> H <sub>23</sub> θ <sub>3</sub> Br	0.5018	(C <sub>6</sub> H <sub>4</sub> CC <sub>6</sub> H <sub>4</sub> ) <sub>2</sub>
0.4235	C <sub>19</sub> H <sub>26</sub> θ <sub>2</sub> N <sub>2</sub>	0.5028	C <sub>17</sub> H <sub>14</sub> θ <sub>6</sub>
0.4237	C <sub>32</sub> H <sub>51</sub> Iθ <sub>2</sub>	0.5034	ClCH <sub>2</sub> CθC <sub>6</sub> H <sub>5</sub>
0.4245	C <sub>21</sub> H <sub>28</sub> θ <sub>5</sub>	0.5065	C <sub>27</sub> H <sub>32</sub> BrNθ <sub>5</sub> •CH <sub>3</sub> θR
0.4255	C <sub>21</sub> H <sub>28</sub> θ <sub>5</sub>	0.5078	C <sub>13</sub> H <sub>12</sub> N <sub>2</sub> θ
0.4284	[CH <sub>3</sub> •Cθθ•θ-C <sub>19</sub> H <sub>28</sub> -CH(CH <sub>3</sub> )CH•CHCH(C <sub>2</sub> H <sub>5</sub> ) CH(CH <sub>3</sub> ) <sub>2</sub> ]	0.5084	C <sub>24</sub> H <sub>35</sub> Brθ <sub>8</sub>
0.4302	(Nθ <sub>2</sub> ) <sub>2</sub> Co(C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> ) <sub>2</sub> Cl	0.5090	C <sub>14</sub> H <sub>18</sub> θ <sub>6</sub> •H <sub>2</sub> θ
0.4310	C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> θ <sub>3</sub> •CH <sub>3</sub> I	0.5118	CH <sub>2</sub> θH(CHθH) <sub>4</sub> CH <sub>2</sub> θH
0.4312	C <sub>23</sub> H <sub>31</sub> IN <sub>2</sub> θ <sub>4</sub>	0.5120	C <sub>15</sub> H <sub>24</sub> θ <sub>2</sub>
0.4313	(C <sub>5</sub> H <sub>5</sub> )Fe(C <sub>5</sub> H <sub>4</sub> •C[ :NθH]C <sub>6</sub> H <sub>5</sub> )	0.5164	C <sub>22</sub> H <sub>25</sub> Brθ <sub>4</sub>
0.4321	C <sub>5</sub> H <sub>5</sub> Nθ	0.5183	C <sub>19</sub> H <sub>30</sub> θ <sub>2</sub>
0.4331	NH <sub>4</sub> Cr(C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> θ <sub>8</sub> )•2H <sub>2</sub> θ	0.5198	C <sub>22</sub> H <sub>26</sub> θ <sub>4</sub>
0.4341	NH <sub>4</sub> Al(C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> θ <sub>8</sub> )•2H <sub>2</sub> θ	0.5214	C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> •CH <sub>3</sub> CθCH <sub>3</sub>
0.4342	C <sub>21</sub> H <sub>26</sub> θ <sub>5</sub>	0.5214	C <sub>18</sub> H <sub>32</sub> θ <sub>16</sub> •5H <sub>2</sub> θ
0.4345	C <sub>25</sub> H <sub>42</sub> N <sub>2</sub> •2HI	0.5230	Cu(C <sub>11</sub> H <sub>14</sub> Nθ) <sub>2</sub>
		0.5234	KC <sub>9</sub> H <sub>4</sub> N <sub>3</sub> θ <sub>2</sub>

$P2_12_12_1$   $D_2^4$  No. 19 (continued)

## Organic (continued)

0.5234	$C_{33}H_{31}Br\theta_4$	0.5902	$C_6H_5\bullet N:N\bullet C_6H_4SCN$
0.5234	$C_{11}H_{17}N_3\theta_8\bullet HBr$	0.5922	$C_5H_9N\theta_3$
0.5258	$(C_6F_5)_2Hg$	0.5922	$C_{26}H_{30}Br\theta_5$
0.5263	$C_{19}H_{22}\theta_{N_2}$	0.5927	$C_{20}H_{26}\theta_2$
0.5274	$C_{24}H_{40}\theta_4\bullet C_2H_5\theta H$	0.5946	$(CH_2CO)_2\theta$
0.5279	$C_{19}H_{32}\theta_2$	0.5967	$C_{23}H_{30}\theta_6$
0.5320	$C_{13}H_9N$	0.5968	$C_{13}H_{18}N_2\theta_4\bullet HBr$
0.5347	$C_6H_{12}\theta_5$	0.5984	$(C_6H_6\theta_2N\bullet NH_2NH)[Cr(NCS)_4(NH_3)_2]_2$
0.5354	$Li\theta H\bullet 3C_6H_{10}\theta_5\bullet 3H_2\theta$	0.5992	$C_{21}H_{34}\theta_5$
0.5364	$C_{10}H_{15}\theta N$	0.6014	$C_{12}H_{14}\theta_3(C\theta C_3H_7)_8$
0.5387	$C_6H_{12}\theta_6$	0.6022	$C_{30}H_{39}I\theta_8$
0.5397	$C_{23}H_{32}\theta_4$	0.6031	$NaI\bullet 2[CH_3CO\bullet NH_2]$
0.5423	$C_{18}H_{22}\theta_2$	0.6038	$C_{22}H_{26}N_3S_2$
0.5439	$C_{27}H_{42}FeN_5\theta_{12}$	0.6050	$NH_2\bullet C_5H_4N$
0.5440	$C_{21}H_{32}\theta_2$	0.6051	$ClCH_2C\theta\theta NH_4$
0.5440	$H\theta C_{18}H_{21}\theta$	0.6055	$C_6H_8\theta_7\bullet H_2\theta$
0.5442	$Na\theta H\bullet 3C_6H_{10}\theta_5\bullet 3H_2\theta$	0.6055	$C_{28}H_{31}BrN_2\theta_4$
0.5443	$Ni(SC(NH_2)_2)_4\bullet S_2\theta_3$	0.6064	$S_7NC\theta CH_3$
0.5451	$C_{30}H_{44}BrN_3\theta_3$	0.6068	$C_9H_{11}FN_2\theta_5$
0.5451	$C_{18}H_{22}\theta_2$	0.6076	$C_{12}H_{14}\theta_{11}(C\theta CH_3)_8$
0.5464	$NiS_2\theta_3\bullet 4(NH_2)_2CS\bullet H_2\theta$	0.6082	$C_4H_4ClN\theta_2$
0.5478	$C_{14}H_{18}\theta_7$	0.6088	$Sr(HCO\theta)_2\bullet 2H_2\theta$
0.5479	$C_7H_{14}\theta_7$	0.6100	$C_6H_8\theta_6(C\theta CH_3)_6$
0.5487	$C_{12}H_7N_4\theta_6I$	0.6104	$C_{11}H_{17}\theta N$
0.5487	$C_8\theta H\bullet 3C_6H_{10}\theta_5\bullet 3H_2\theta$	0.6106	$C_{14}H_{18}\theta_6$
0.5498	$C_{21}H_{30}\theta_2$	0.6113	$Ni(C_2H_4\theta NS)_2$
0.5508	$C_6H_{12}\theta_5$	0.6113	$C_4H_4BrN\theta_2$
0.5532	$C_{21}H_{30}\theta_3\bullet CH_3CO\theta$	0.6125	$C_8H_{18}BrN\theta$
0.5572	$C_{11}H_{17}\theta N\bullet HBr$	0.6133	$C_6H_{12}\theta_6$
0.5572	$C_{19}H_{29}N\theta_2\bullet HI$	0.6136	$C_6H_{12}\theta_6$
0.5582	$C_6H_{10}\theta_5$	0.6182	$C_{10}H_{8}\theta_3$
0.5590	$C_{25}H_{28}\theta_3$	0.6188	$[(N\theta)_2]_3C_6H_2]_2NH$
0.5599	$C_{19}H_{27}Br\theta_2$	0.6192	$C_6H_7\theta(C\theta\theta CH_3)_5$
0.5600	$C_6H_7\theta(C\theta\theta CH_3)_5$	0.6206	$C_{22}H_{32}\theta_3$
0.5619	$NH_4\theta H\bullet 3C_6H_{10}\theta_5\bullet 3H_2\theta$	0.6206	$C_6H_{11}\theta_5(CH_3)$
0.5619	$K\theta H\bullet 3C_6H_{10}\theta_5\bullet 3H_2\theta$	0.6214	$(C_5H_5)Fe(C_5H_4\bullet C\theta\theta C_2H_5)$
0.5625	$C_{22}H_{17}IN_2\theta_5$	0.6230	$C_6H_8\theta_6(CH_3)_4$
0.5630	$(C_5H_5)Fe(C_5H_4\bullet C\theta\theta C_6H_4\bullet\theta H)$	0.6236	$C_7\theta_3NH_7$
0.5632	$C_7H_{14}\theta_7$	0.6237	$C_{21}H_{36}\theta_4$
0.5635	$C_6H_6ClN$	0.6240	$C_6H_9\theta_7\bullet NH_4\bullet H_2\theta$
0.5637	$C_{26}H_{31}N\theta_5\bullet HBr$	0.6242	$C_{16}H_{21}N\theta_3\bullet HI$
0.5639	$C_{18}H_{23}\theta_2Br\bullet CH_3\theta H$	0.6265	$C_{21}H_{36}\theta_2$
0.5675	$N\theta_2\bullet C_6H_4\bullet N_3$	0.6275	$C_{17}H_{19}\theta_3N\bullet HCl\bullet 3H_2\theta$
0.5677	$C_6H_{10}\theta_5$	0.6285	$C_{18}H_{21}N\theta_3\bullet HBr\bullet 2H_2\theta$
0.5683	$C_{15}H_{25}Br$	0.6286	$C_{18}H_{21}N\theta_3HI\bullet 2H_2\theta$
0.5685	$C_4H_9\theta_3N$	0.6287	$C_{20}H_{26}\theta_2$
0.5687	$C_{16}H_{21}N\theta_3\bullet HBr$	0.6298	$C_4H_4Ca\theta_5\bullet 2H_2\theta$
0.5690	$Ca(C_6H_9\theta_7)_2\bullet 3H_2\theta$	0.6314	$C_{46}H_{58}\theta_{13}N_6CoCl\bullet 2H_2\theta\bullet CH_3C\theta\theta CH_3$
0.5696	$C_{27}H_{45}N\theta_2\bullet HBr$	0.6317	$C_{18}H_{21}\theta_3N\bullet HCl\bullet 2H_2\theta$
0.5716	$C_{11}H_{17}\theta N\bullet HCl$	0.6331	$C_{22}H_{29}I\theta_6$
0.5717	$C_{30}H_{47}Br\theta$	0.6335	$C_{10}H_{16}Br_2\theta$
0.5720	$NH_2\bullet C\theta\theta\bullet NHNH_2\bullet HCl$	0.6344	$C_{18}H_{14}$
0.5725	$C_{22}H_{31}IN_2\theta$	0.6353	$C_{17}H_{19}N\theta_3\bullet HBr\bullet 2H_2\theta$
0.5731	$C_{21}H_{27}Cl\theta_2$	0.6390	$C_6H_5N:NC_6H_4S_2C_6H_4N:NC_6H_5$
0.5742	$C_6H_5-(CH\theta H)_2-C\theta\theta H$	0.6393	$C_4H_2\theta_3$
0.5746	$C_{17}H_{23}Br\theta_5$	0.6399	$C_8H_{15}\theta_2SN\bullet HCl\bullet H_2\theta$
0.5760	$C_6H_5(NH_2CSNH_2)_2TeCl$	0.6400	$MgC\theta_3\bullet 3H_2\theta$
0.5760	$C_{20}H_{27}BrN_2\theta$	0.6400	$C_{15}H_{25}Cl$
0.5763	$C_{19}H_{26}\theta_2\bullet C_6H_5\theta Br$	0.6407	$C_{17}H_{15}N\theta_3\bullet HI\bullet 2H_2\theta$
0.5772	$C_{30}H_{50}Cr\theta_4$	0.6407	$C_{19}H_{24}\theta_2$
0.5773	$C_{16}H_{10}N_2\theta_2$	0.6408	$C_{33}H_{51}\theta_4I$
0.5778	$C_{21}H_{27}Br\theta_2$	0.6409	$C_{34}H_{51}I\theta_6$
0.5784	$C_{15}H_{20}\theta_3$	0.6420	$K(C_{10}H_{16}\theta_9NS_2)\bullet H_2\theta$
0.5788	$C_{16}H_{24}\theta_4$	0.6420	$C_{16}H_{21}N\theta_3\bullet HBr$
0.5796	$C(NH_2)_3\theta H\bullet 3C_6H_{10}\theta_5\bullet 3H_2\theta$	0.6438	$(C_6H_{10}\theta_5)_n$
0.5807	$C_6H_9N_3\theta_2\bullet HCl\bullet H_2\theta$	0.6449	$C_{20}H_{32}$
0.5809	$C_{15}H_{20}\theta_6$	0.6454	$C_{20}H_{23}Br\theta_6$
0.5815	$C_{20}H_{27}N_2\theta Cl$	0.6471	$C_{22}H_{25}N\theta_6\bullet CH_3I$
0.5820	$C_{20}H_{27}IN_2\theta_2$	0.6507	$(CH_3)_3N\bullet C_2H_4\bullet\theta\theta CCH_3Cl$
0.5834	$C_{17}H_{16}CuN_2\theta_2\bullet H_2\theta$	0.6523	$H_2N-C_6H_4\bullet S\theta_2\bullet NH\bullet C\theta\theta\bullet NH\bullet C_4H_9$
0.5851	$C_{20}H_{27}IN_2\theta_2$	0.6550	$C_{28}H_{30}INP_2$
0.5853	$C_{15}H_{25}Cl$	0.6551	$C_{15}H_{25}Br$
0.5871	$C_{27}H_{44}\theta$	0.6570	$C_9H_{13}\theta_7N_3Cu\bullet H_2\theta$

P2<sub>1</sub>2<sub>1</sub><sup>2</sup><sub>1</sub> D<sub>2</sub><sup>4</sup> No. 19 (continued)

## Organic (continued)

0.6581	C <sub>21</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub> •CH <sub>3</sub> I	0.7496	C <sub>22</sub> H <sub>29</sub> IN <sub>2</sub> O <sub>4</sub>
0.6581	BrC <sub>6</sub> H <sub>2</sub> (C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> OH	0.7521	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>
0.6619	CH <sub>3</sub> C <sub>6</sub> H <sub>2</sub> (C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> OH	0.7541	(H <sub>2</sub> N) <sub>2</sub> C•NH(CH <sub>2</sub> ) <sub>3</sub> CH•NH <sub>2</sub> •C <sub>6</sub> H <sub>5</sub> •2H <sub>2</sub> O
0.6622	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	0.7547	C <sub>16</sub> H <sub>9</sub> N <sub>2</sub> O <sub>2</sub> Br
0.6645	C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>	0.7560	C <sub>8</sub> H <sub>17</sub> O•HCl
0.6653	C <sub>19</sub> H <sub>17</sub> N•C <sub>2</sub> H <sub>5</sub> (OH) <sub>4</sub> •(CH <sub>3</sub> ) <sub>3</sub> •HI•3H <sub>2</sub> O	0.7564	C <sub>23</sub> H <sub>34</sub> O <sub>3</sub>
0.6662	C <sub>4</sub> H <sub>8</sub> •PtCl <sub>2</sub> •NH <sub>2</sub> CH(CH <sub>3</sub> )C <sub>6</sub> H <sub>5</sub>	0.7567	C <sub>39</sub> H <sub>39</sub> Br <sub>6</sub> S
0.6668	C <sub>30</sub> H <sub>49</sub> O•C <sub>6</sub> H <sub>5</sub> I	0.7579	As <sub>2</sub> C <sub>14</sub> H <sub>14</sub> Br <sub>2</sub>
0.6684	[(NO <sub>2</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>2</sub> ] <sub>2</sub> NNa	0.7580	C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>
0.6712	C <sub>11</sub> H <sub>8</sub> N <sub>2</sub>	0.7580	C <sub>19</sub> H <sub>27</sub> Br <sub>2</sub> O
0.6718	C <sub>8</sub> H <sub>13</sub> O•HCl	0.7582	C <sub>26</sub> H <sub>30</sub> O <sub>8</sub> •CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub>
0.6740	[C <sub>19</sub> H <sub>28</sub> Br <sub>3</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> ]	0.7601	C <sub>10</sub> H <sub>6</sub> (NO <sub>2</sub> ) <sub>2</sub>
0.6749	C <sub>14</sub> H <sub>15</sub> Br <sub>2</sub> O <sub>3</sub>	0.7604	[C <sub>19</sub> H <sub>29</sub> -CH(CH <sub>3</sub> )CH <sub>2</sub> CF <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub> •HCl]
0.6775	C <sub>40</sub> H <sub>44</sub> I <sub>2</sub> N <sub>4</sub> O <sub>2</sub>	0.7605	C <sub>6</sub> H <sub>5</sub> •CH <sub>2</sub> O•C <sub>6</sub> H <sub>5</sub> •NH•CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> •NH•CH(CH <sub>3</sub> )C <sub>6</sub> H <sub>5</sub> •C <sub>2</sub> H <sub>5</sub> O
0.6799	C <sub>21</sub> H <sub>36</sub> O <sub>2</sub>	0.7630	C <sub>9</sub> H <sub>20</sub> O <sub>2</sub> NI
0.6809	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub>	0.7645	CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N=C=NC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub>
0.6821	C <sub>11</sub> H <sub>14</sub> BrN <sub>3</sub> O <sub>7</sub> •HBr	0.7647	C <sub>21</sub> H <sub>26</sub> O <sub>3</sub> N <sub>2</sub>
0.6822	C <sub>6</sub> H <sub>9</sub> K <sub>6</sub> O <sub>7</sub> •2H <sub>2</sub> O	0.7657	C <sub>19</sub> H <sub>26</sub> O <sub>2</sub>
0.6835	C <sub>14</sub> H <sub>21</sub> Br <sub>2</sub> O <sub>3</sub>	0.7659	C <sub>34</sub> H <sub>47</sub> O <sub>11</sub> N•HBr•4H <sub>2</sub> O
0.6839	C <sub>5</sub> H <sub>5</sub> N <sub>6</sub> •HCl	0.7659	C <sub>34</sub> H <sub>47</sub> O <sub>11</sub> N•HCl•xH <sub>2</sub> O
0.6882	AlH <sub>3</sub> •[(CH <sub>3</sub> ) <sub>2</sub> N•CH <sub>2</sub> CH <sub>2</sub> •N(CH <sub>3</sub> ) <sub>2</sub> ]	0.7666	[(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> ][B(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> ]
0.6893	C <sub>10</sub> H <sub>9</sub> Cl <sub>4</sub> S <sub>2</sub>	0.7672	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> BiCl <sub>2</sub>
0.6904	C <sub>5</sub> H <sub>5</sub> N <sub>6</sub> •HBr	0.7672	C <sub>23</sub> H <sub>31</sub> O <sub>2</sub> (OH) <sub>3</sub>
0.6948	C <sub>24</sub> H <sub>24</sub> IN <sub>3</sub> O <sub>5</sub> •C <sub>2</sub> H <sub>5</sub> OH	0.7675	C <sub>34</sub> H <sub>47</sub> O <sub>11</sub> N•HI•xH <sub>2</sub> O
0.6956	C <sub>27</sub> H <sub>45</sub> N <sub>6</sub> •HI	0.7686	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>6</sub> •H <sub>2</sub> O
0.6961	C <sub>21</sub> H <sub>30</sub> O <sub>3</sub>	0.7687	C <sub>6</sub> H <sub>7</sub> N <sub>3</sub> O
0.6962	C <sub>5</sub> H <sub>5</sub> N <sub>6</sub> •HCl	0.7688	C <sub>6</sub> H <sub>12</sub> O <sub>3</sub> S
0.6972	C <sub>14</sub> H <sub>16</sub> O <sub>3</sub>	0.7694	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub>
0.6981	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	0.7696	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>3</sub> CF <sub>2</sub> Fe(C <sub>6</sub> ) <sub>3</sub>
0.6984	C <sub>6</sub> H <sub>5</sub> As <sub>2</sub> (OH) <sub>2</sub>	0.7703	C <sub>42</sub> H <sub>47</sub> I <sub>3</sub> O <sub>8</sub>
0.7021	B <sub>10</sub> H <sub>13</sub> C <sub>2</sub> H <sub>5</sub>	0.7704	C <sub>42</sub> H <sub>47</sub> Br <sub>3</sub> O <sub>8</sub>
0.7025	C <sub>22</sub> H <sub>27</sub> IN <sub>2</sub> O <sub>3</sub> •xH <sub>2</sub> O	0.7738	C <sub>16</sub> H <sub>15</sub> Br
0.7038	C <sub>11</sub> H <sub>14</sub> N <sub>3</sub> O <sub>7</sub> •HCl•H <sub>2</sub> O	0.7758	C <sub>34</sub> H <sub>38</sub> IN <sub>2</sub> O <sub>12</sub> •x(C <sub>3</sub> H <sub>6</sub> O)
0.7042	C <sub>6</sub> H <sub>5</sub> As <sub>2</sub> (OH) <sub>2</sub>	0.7762	(C <sub>8</sub> H <sub>8</sub> N <sub>6</sub> ) <sub>2</sub> Cu
0.7045	C <sub>21</sub> H <sub>30</sub> O <sub>3</sub>	0.7770	C <sub>26</sub> H <sub>30</sub> O <sub>8</sub> CH <sub>3</sub> OH
0.7084	C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub> •H <sub>2</sub> O	0.7773	C <sub>34</sub> H <sub>24</sub>
0.7085	C <sub>12</sub> H <sub>19</sub> Br <sub>2</sub> O	0.7773	C <sub>32</sub> H <sub>46</sub> O <sub>7</sub>
0.7087	NH <sub>4</sub> •H•(H <sub>6</sub> C•CH•C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.7775	C <sub>4</sub> NH <sub>8</sub> C <sub>6</sub> H <sub>5</sub>
0.7093	LiCl•C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	0.7794	Co(C <sub>3</sub> HNH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub>
0.7098	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub>	0.7798	(OH) <sub>2</sub> (CH <sub>3</sub> ) <sub>4</sub> CH <sub>2</sub> Si <sub>2</sub>
0.7122	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> PON(CH <sub>3</sub> ) <sub>2</sub>	0.7809	C <sub>4</sub> H <sub>7</sub> (NH) <sub>2</sub> C <sub>6</sub> H <sub>5</sub>
0.7133	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> •P <sub>2</sub> O <sub>5</sub> •CH <sub>3</sub>	0.7820	C <sub>15</sub> H <sub>15</sub> O <sub>6</sub> Cl
0.7143	[Cu(NH <sub>2</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ] <sub>2</sub> •H <sub>2</sub> O	0.7832	C <sub>4</sub> H <sub>4</sub> Na <sub>2</sub> O <sub>6</sub> •2H <sub>2</sub> O
0.7144	C <sub>6</sub> H <sub>6</sub> K <sub>5</sub>	0.7872	C <sub>18</sub> H <sub>12</sub>
0.7145	CH <sub>3</sub> C(N <sub>6</sub> H) <sub>2</sub>	0.7872	(CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> C <sub>6</sub> H <sub>8</sub> O <sub>5</sub> (C <sub>6</sub> H <sub>4</sub> N <sub>4</sub> O <sub>4</sub> )
0.7152	C <sub>6</sub> H <sub>7</sub> O <sub>5</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub>	0.7881	Cu(C <sub>6</sub> H <sub>18</sub> N <sub>4</sub> )(SCN)(NCS)
0.7210	C <sub>4</sub> H <sub>5</sub> O <sub>6</sub> Rb	0.7889	C <sub>22</sub> H <sub>27</sub> N <sub>2</sub> O•HCl•H <sub>2</sub> O
0.7258	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ICl•HgCl <sub>2</sub>	0.7892	C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub> C <sub>2</sub> H <sub>6</sub> O
0.7261	CH <sub>3</sub> CHBrC <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> •NHCH <sub>2</sub> C <sub>6</sub> H <sub>5</sub>	0.7901	C <sub>14</sub> H <sub>18</sub> IN <sub>2</sub> O
0.7265	C <sub>26</sub> H <sub>16</sub>	0.7910	C <sub>10</sub> H <sub>19</sub> N(CH <sub>3</sub> ) <sub>3</sub> I
0.7271	C <sub>6</sub> H <sub>6</sub> H <sub>5</sub> Rb	0.7929	C <sub>6</sub> H <sub>10</sub> O <sub>6</sub>
0.7278	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>	0.7929	C <sub>22</sub> H <sub>27</sub> IN <sub>2</sub> O <sub>3</sub>
0.7280	C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O	0.7952	C <sub>19</sub> H <sub>24</sub> O <sub>2</sub> N <sub>2</sub> •HCl•H <sub>2</sub> O
0.7286	C <sub>5</sub> H <sub>6</sub> O <sub>5</sub> (CH <sub>3</sub> ) <sub>3</sub>	0.7966	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>6</sub> •HCl
0.7288	C <sub>12</sub> H <sub>14</sub> O <sub>3</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>8</sub>	0.7971	C <sub>29</sub> H <sub>21</sub> Br <sub>6</sub> O <sub>11</sub>
0.7292	C <sub>10</sub> H <sub>15</sub> O•N•HI	0.8020	C <sub>22</sub> H <sub>25</sub> N <sub>6</sub> O <sub>6</sub> CH <sub>2</sub> Br <sub>2</sub>
0.7298	(CH <sub>3</sub> CH <sub>2</sub> •C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> KH	0.8048	Cu(NH <sub>2</sub> •CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •H <sub>2</sub> O
0.7300	C <sub>16</sub> H <sub>21</sub> N <sub>6</sub> O <sub>3</sub>	0.8057	C <sub>22</sub> H <sub>25</sub> N <sub>6</sub> O <sub>6</sub> •CH <sub>2</sub> I <sub>2</sub>
0.7302	C <sub>20</sub> H <sub>24</sub> O <sub>3</sub>	0.8076	C <sub>20</sub> H <sub>24</sub> N <sub>2</sub> O <sub>2</sub> •0.25C <sub>6</sub> H <sub>6</sub>
0.7329	C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> •H <sub>2</sub> O	0.8089	H <sub>6</sub> C•C <sub>6</sub> H <sub>5</sub> •C <sub>6</sub> H <sub>5</sub>
0.7336	C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> •HCl	0.8101	C <sub>10</sub> H <sub>17</sub> Br <sub>2</sub> O
0.7343	B <sub>10</sub> H <sub>10</sub> (CCH <sub>2</sub> Br) <sub>2</sub>	0.8118	C <sub>26</sub> H <sub>34</sub> O <sub>6</sub>
0.7344	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	0.8119	C <sub>6</sub> H <sub>8</sub> O <sub>6</sub> (CH <sub>3</sub> ) <sub>4</sub>
0.7352	NIN(CH <sub>2</sub> •CH <sub>2</sub> •NH <sub>2</sub> ) <sub>3</sub> (SCN) <sub>2</sub>	0.8137	C <sub>10</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> •H <sub>2</sub> O
0.7365	C <sub>24</sub> H <sub>36</sub> O <sub>3</sub>	0.8139	C <sub>6</sub> H <sub>4</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> Te)
0.7380	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>	0.8139	Zn(O <sub>6</sub> C•CH <sub>2</sub> •CH(NH <sub>2</sub> )•C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> •H <sub>2</sub> O
0.7391	C <sub>6</sub> H <sub>11</sub> O <sub>6</sub> CH <sub>3</sub>	0.8146	C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub> S <sub>3</sub>
0.7405	C <sub>16</sub> H <sub>17</sub> O•N <sub>3</sub> •CH <sub>3</sub> OH	0.8149	C <sub>16</sub> H <sub>25</sub> N <sub>6</sub> •HBr
0.7449	C <sub>14</sub> H <sub>22</sub> O <sub>4</sub> N <sub>2</sub> S	0.8159	C <sub>22</sub> H <sub>28</sub> N <sub>4</sub> Cl <sub>2</sub> •2H <sub>2</sub> O
0.7451	C <sub>33</sub> H <sub>51</sub> N <sub>6</sub> O	0.8165	C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub> O <sub>2</sub>
0.7460	C <sub>6</sub> H <sub>3</sub> (OH) <sub>3</sub>	0.8180	C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O
0.7463	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	0.8185	C <sub>26</sub> H <sub>30</sub> O <sub>8</sub>
0.7463	H <sub>6</sub> C <sub>18</sub> H <sub>21</sub> O	0.8188	NaHC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> •H <sub>2</sub> O
0.7465	C <sub>6</sub> N <sub>2</sub> O <sub>3</sub> H <sub>15</sub> •HBr	0.8213	C <sub>15</sub> H <sub>10</sub> O



P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub> D<sub>2</sub><sup>4</sup> No. 19 (continued)

## Organic (continued)

0.8223	C <sub>27</sub> H <sub>44</sub>	0.8852	C <sub>45</sub> H <sub>55</sub> BrN <sub>2</sub> Cl <sub>3</sub>
0.8224	C <sub>10</sub> H <sub>16</sub> BrN <sub>2</sub>	0.8852	C <sub>5</sub> H <sub>5</sub> Cl <sub>5</sub> (CH <sub>3</sub> ) <sub>3</sub>
0.8235	C <sub>12</sub> H <sub>14</sub> Cl <sub>3</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>8</sub>	0.8864	C <sub>32</sub> H <sub>49</sub> Cl <sub>3</sub>
0.8242	I(CH <sub>3</sub> ) <sub>4</sub> C <sub>6</sub> H	0.8872	C <sub>5</sub> H <sub>9</sub> Cl <sub>4</sub> NHCl
0.8242	BrC <sub>6</sub> H(CH <sub>3</sub> ) <sub>4</sub>	0.8873	C <sub>16</sub> H <sub>22</sub> Cl <sub>3</sub> NBr
0.8242	C <sub>28</sub> H <sub>39</sub> BrCl <sub>9</sub>	0.8877	H <sub>2</sub> C <sub>3</sub> P <sub>2</sub> CH <sub>2</sub> CH(NH <sub>3</sub> )C <sub>6</sub> H <sub>5</sub>
0.8243	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> Cl <sub>4</sub>	0.8909	C <sub>23</sub> H <sub>24</sub> Br <sub>2</sub> N <sub>4</sub> Cl <sub>3</sub> S
0.8246	C <sub>23</sub> H <sub>32</sub> Cl <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.8911	C <sub>5</sub> H <sub>6</sub> Cl <sub>5</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub>
0.8257	C <sub>16</sub> H <sub>19</sub> N <sub>2</sub> Cl <sub>4</sub> •HBr	0.8943	C <sub>18</sub> H <sub>24</sub> N <sub>2</sub> Cl <sub>3</sub>
0.8258	C <sub>6</sub> N <sub>2</sub> NHCH <sub>3</sub>	0.8949	C <sub>63</sub> H <sub>88</sub> CoN <sub>14</sub> Cl <sub>14</sub> PSe
0.8259	Co[ClC <sub>6</sub> CH <sub>2</sub> •CH(NH <sub>2</sub> )•C <sub>6</sub> H <sub>5</sub> ] <sub>3</sub> •3H <sub>2</sub> O	0.8951	C <sub>45</sub> H <sub>55</sub> IN <sub>2</sub> Cl <sub>3</sub>
0.8267	C <sub>10</sub> H <sub>19</sub> N(CH <sub>3</sub> ) <sub>3</sub> I	0.8954	H <sub>2</sub> N•CH <sub>2</sub> N <sub>2</sub> H
0.8282	Ni[ClC <sub>6</sub> CH <sub>2</sub> •CH(NH <sub>2</sub> )•C <sub>6</sub> H <sub>5</sub> ] <sub>3</sub> •3H <sub>2</sub> O	0.8954	C <sub>24</sub> H <sub>35</sub> N <sub>2</sub> Cl <sub>4</sub> •HI
0.8300	C <sub>9</sub> H <sub>6</sub> Cl <sub>3</sub> •H <sub>2</sub> O	0.8990	C <sub>18</sub> H <sub>34</sub> N <sub>2</sub> Cl <sub>3</sub> •S•HCl•H <sub>2</sub> O
0.8307	(CH <sub>3</sub> SCl <sub>2</sub> ) <sub>2</sub> C=C=N(C <sub>2</sub> H <sub>5</sub> )	0.8997	C <sub>26</sub> H <sub>32</sub> Cl <sub>6</sub>
0.8307	C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> Cl <sub>4</sub> •HBr•H <sub>2</sub> O	0.8999	C <sub>13</sub> H <sub>14</sub> Cl <sub>5</sub>
0.8308	Sr(CH <sub>2</sub> ) <sub>2</sub>	0.9003	C <sub>13</sub> H <sub>10</sub> Cl <sub>10</sub>
0.8318	NH <sub>2</sub> C <sub>6</sub> CH <sub>2</sub> •CH(NH <sub>2</sub> )C <sub>6</sub> H <sub>5</sub> •H <sub>2</sub> O	0.9003	C <sub>62</sub> H <sub>89</sub> CoN <sub>13</sub> Cl <sub>15</sub> P
0.8326	C <sub>22</sub> H <sub>26</sub> N <sub>4</sub> •2HBr•2H <sub>2</sub> O	0.9035	C <sub>11</sub> H <sub>21</sub> N <sub>3</sub> Cl <sub>4</sub>
0.8332	C <sub>22</sub> H <sub>23</sub> N <sub>2</sub> Cl <sub>8</sub> •HCl	0.9035	C <sub>17</sub> H <sub>21</sub> BrCl <sub>5</sub>
0.8341	C <sub>18</sub> H <sub>21</sub> BrCl <sub>2</sub>	0.9036	C <sub>40</sub> H <sub>59</sub> Cl <sub>10</sub> N <sub>8</sub> I
0.8360	C <sub>15</sub> H <sub>23</sub> Cl <sub>2</sub> N <sub>2</sub> SeCl <sub>4</sub>	0.9066	C <sub>6</sub> H <sub>12</sub> Cl <sub>6</sub>
0.8370	C <sub>12</sub> H <sub>14</sub> Cl <sub>11</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>8</sub>	0.9074	C <sub>6</sub> H <sub>12</sub> Se <sub>3</sub>
0.8376	Cu(C <sub>5</sub> H <sub>5</sub> N) <sub>4</sub> (BF <sub>4</sub> ) <sub>2</sub>	0.9091	C <sub>27</sub> H <sub>41</sub> NCl <sub>7</sub>
0.8389	C <sub>7</sub> H <sub>7</sub> V(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub>	0.9095	C <sub>21</sub> H <sub>30</sub> Cl <sub>2</sub>
0.8394	C <sub>9</sub> H <sub>13</sub> Cl <sub>6</sub>	0.9096	C <sub>9</sub> H <sub>6</sub> N <sub>2</sub>
0.8427	C <sub>6</sub> H <sub>9</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub>	0.9105	C <sub>20</sub> H <sub>27</sub> IN <sub>2</sub>
0.8439	C <sub>9</sub> H <sub>13</sub> BrCl	0.9117	C <sub>11</sub> H <sub>10</sub> N <sub>2</sub>
0.8461	Pb(HCl <sub>2</sub> ) <sub>2</sub>	0.9126	C <sub>26</sub> H <sub>31</sub> N <sub>2</sub> Cl <sub>3</sub> I
0.8474	C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> Cl <sub>4</sub> Na•H <sub>2</sub> O	0.9127	CaC <sub>4</sub> H <sub>4</sub> Cl <sub>6</sub> •4H <sub>2</sub> O
0.8475	C <sub>25</sub> H <sub>32</sub> IN <sub>3</sub> Cl <sub>4</sub> •H <sub>2</sub> O	0.9133	C <sub>29</sub> H <sub>32</sub> BrN <sub>2</sub> Cl <sub>9</sub>
0.8477	C <sub>30</sub> H <sub>39</sub> BrCl <sub>4</sub>	0.9133	C <sub>14</sub> H <sub>10</sub> Cl <sub>6</sub> (N <sub>2</sub> Cl <sub>2</sub> ) <sub>3</sub>
0.8482	C <sub>15</sub> H <sub>23</sub> Cl <sub>2</sub> N <sub>2</sub> SeCl <sub>4</sub>	0.9145	C <sub>33</sub> H <sub>37</sub> I <sub>2</sub> Cl <sub>11</sub> SeCl <sub>3</sub> H <sub>6</sub> Cl
0.8484	C <sub>2</sub> H <sub>4</sub> •ClPt•NH <sub>2</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub>	0.9153	C <sub>30</sub> H <sub>42</sub> Cl <sub>2</sub> N <sub>2</sub> Se•2HBr•4H <sub>2</sub> O
0.8495	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> •CH <sub>2</sub> •CH(NH <sub>2</sub> )•C <sub>6</sub> H <sub>5</sub>	0.9172	C <sub>22</sub> H <sub>26</sub> N <sub>4</sub>
0.8502	C <sub>5</sub> H <sub>9</sub> P <sub>2</sub> Br <sub>2</sub>	0.9192	C <sub>30</sub> H <sub>28</sub> CuN <sub>2</sub> Cl <sub>2</sub>
0.8505	C <sub>6</sub> H <sub>5</sub> Cl <sub>6</sub> N <sub>2</sub>	0.9205	C <sub>6</sub> H <sub>4</sub> •CBr•CCH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub>
0.8508	C <sub>13</sub> H <sub>16</sub> I <sub>2</sub> N <sub>5</sub>	0.9222	C <sub>12</sub> H <sub>15</sub> IN <sub>2</sub> Cl <sub>3</sub>
0.8509	H <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> NH(CH <sub>2</sub> ) <sub>2</sub> NH <sub>2</sub> •C <sub>6</sub> H <sub>5</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub>	0.9255	[(NH <sub>2</sub> ) <sub>2</sub> CNHCH <sub>3</sub> ] <sub>2</sub> SeCl <sub>4</sub>
0.8519	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> Cl <sub>5</sub>	0.9256	C <sub>5</sub> H <sub>10</sub> Cl <sub>5</sub>
0.8534	(C <sub>2</sub> H <sub>5</sub> Cl)(CH <sub>3</sub> ) <sub>2</sub> C•Cl(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> HgSCN	0.9275	CH <sub>3</sub> Cl <sub>18</sub> H <sub>20</sub> Br
0.8549	C <sub>4</sub> H <sub>16</sub> I <sub>2</sub> N <sub>4</sub> Ni•H <sub>2</sub> O	0.9286	Co(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> (CH <sub>2</sub> ) <sub>2</sub> CHNH <sub>2</sub> •3H <sub>2</sub> O
0.8578	C <sub>3</sub> H <sub>6</sub> Cl <sub>3</sub> S	0.9289	C <sub>15</sub> H <sub>26</sub> Br <sub>2</sub>
0.8600	C <sub>63</sub> H <sub>88</sub> CoN <sub>14</sub> Cl <sub>14</sub> PS	0.9291	C <sub>18</sub> H <sub>21</sub> NCl <sub>3</sub>
0.8602	C <sub>30</sub> H <sub>38</sub> ClI <sub>2</sub> Cl <sub>8</sub>	0.9294	C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> Cl <sub>4</sub> S
0.8605	C <sub>44</sub> H <sub>28</sub> N <sub>4</sub> Zn	0.9297	C <sub>45</sub> H <sub>53</sub> IN <sub>2</sub> Cl <sub>13</sub> •C <sub>3</sub> H <sub>6</sub> Cl <sub>5</sub> •5H <sub>2</sub> O
0.8616	C <sub>62</sub> H <sub>89</sub> CoN <sub>13</sub> Cl <sub>15</sub> P	0.9316	C <sub>17</sub> H <sub>15</sub> BrN <sub>2</sub>
0.8623	C <sub>16</sub> H <sub>13</sub> Br	0.9324	C <sub>15</sub> H <sub>17</sub> BrCl <sub>4</sub>
0.8639	Ba(ClC <sub>6</sub> H <sub>4</sub> ) <sub>2</sub>	0.9331	C <sub>22</sub> H <sub>29</sub> N <sub>2</sub> Cl <sub>2</sub> •HCl
0.8646	C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> Cl	0.9340	Cu(ClC <sub>6</sub> CH <sub>2</sub> •CH <sub>2</sub> •CHNH <sub>2</sub> •C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •2H <sub>2</sub> O
0.8652	C <sub>63</sub> H <sub>88</sub> CoN <sub>14</sub> Cl <sub>14</sub> PS	0.9350	Zn(ClC <sub>6</sub> CH <sub>2</sub> CH <sub>2</sub> CH(NH <sub>2</sub> )C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •2H <sub>2</sub> O
0.8657	C <sub>15</sub> H <sub>15</sub> BrCl <sub>6</sub>	0.9352	C <sub>37</sub> H <sub>68</sub> IN <sub>2</sub> Cl <sub>13</sub> •2H <sub>2</sub> O
0.8658	C <sub>22</sub> H <sub>29</sub> Cl <sub>4</sub> N <sub>2</sub> Cl	0.9358	C <sub>5</sub> H <sub>10</sub> Cl <sub>4</sub>
0.8679	C <sub>9</sub> H <sub>16</sub> N <sub>4</sub> Cl <sub>5</sub>	0.9367	C <sub>18</sub> H <sub>16</sub> Cl <sub>7</sub>
0.8687	C <sub>13</sub> H <sub>15</sub> N <sub>2</sub> Cl <sub>2</sub> •HBr	0.9375	C <sub>16</sub> H <sub>18</sub> Cl <sub>4</sub> N <sub>2</sub> S
0.8689	C <sub>15</sub> H <sub>15</sub> Cl <sub>6</sub> Br	0.9380	C <sub>12</sub> H <sub>14</sub> Cl <sub>11</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>8</sub>
0.8718	C <sub>5</sub> H <sub>9</sub> Cl <sub>4</sub> N•HBr	0.9380	C <sub>34</sub> H <sub>37</sub> I <sub>2</sub> Cl <sub>9</sub>
0.8718	C <sub>12</sub> H <sub>10</sub> N <sub>2</sub>	0.9389	C <sub>6</sub> H <sub>11</sub> Cl <sub>6</sub> CH <sub>3</sub>
0.8720	C <sub>62</sub> H <sub>88</sub> CoN <sub>14</sub> Cl <sub>14</sub> PS	0.9393	C <sub>7</sub> H <sub>7</sub> N <sub>2</sub>
0.8726	(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> Ni <sub>2</sub> •C <sub>6</sub> H <sub>5</sub> C•C•CC <sub>6</sub> H <sub>5</sub> •Ni <sub>2</sub> (C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub>	0.9400	C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> N <sub>2</sub> •HCl
0.8737	C <sub>18</sub> H <sub>19</sub> Cl <sub>3</sub> N•HBr	0.9408	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> SbCl <sub>2</sub>
0.8743	C <sub>63</sub> H <sub>88</sub> Cl <sub>14</sub> N <sub>14</sub> PCo•18H <sub>2</sub> O	0.9415	(C <sub>10</sub> H <sub>18</sub> N)(C <sub>7</sub> H <sub>7</sub> S <sub>2</sub> Cl <sub>3</sub> )
0.8750	C <sub>7</sub> H <sub>13</sub> ClHgCl <sub>5</sub>	0.9417	C <sub>30</sub> H <sub>46</sub> N <sub>6</sub> Cl <sub>5</sub> •HI•xH <sub>2</sub> O
0.8759	C <sub>63</sub> H <sub>88</sub> CoN <sub>14</sub> Cl <sub>14</sub> PS	0.9442	(C <sub>4</sub> H <sub>8</sub> )(C <sub>6</sub> H <sub>5</sub> CHCH <sub>3</sub> NH <sub>2</sub> )(C <sub>6</sub> H <sub>12</sub> )PtCl <sub>2</sub>
0.8765	(CH <sub>3</sub> )(C <sub>3</sub> H <sub>7</sub> )(C <sub>6</sub> H <sub>5</sub> )(CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> )PBr	0.9454	C <sub>24</sub> H <sub>31</sub> BrCl <sub>8</sub>
0.8765	C <sub>61</sub> H <sub>82</sub> Cl <sub>2</sub> CoN <sub>14</sub> Cl <sub>14</sub> P	0.9462	C <sub>9</sub> H <sub>13</sub> Cl <sub>5</sub> N <sub>3</sub>
0.8766	C <sub>40</sub> H <sub>48</sub> I <sub>2</sub> N <sub>4</sub> Cl <sub>2</sub> •nH <sub>2</sub> O	0.9465	(CH <sub>3</sub> ) <sub>3</sub> (C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> )Pt
0.8766	C <sub>5</sub> H <sub>9</sub> Cl <sub>5</sub> SNCu•2H <sub>2</sub> O	0.9466	(C <sub>6</sub> H <sub>2</sub> )(N <sub>2</sub> ) <sub>4</sub>
0.8780	[(C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> P] <sub>3</sub> (CdBr <sub>2</sub> ) <sub>2</sub>	0.9469	C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub>
0.8786	C <sub>7</sub> H <sub>5</sub> BrCl <sub>2</sub>	0.9483	C <sub>20</sub> H <sub>14</sub> CuN <sub>2</sub> Cl <sub>2</sub>
0.8810	C <sub>6</sub> H <sub>4</sub> •CHCl(CN)•C <sub>6</sub> H <sub>4</sub>	0.9483	C <sub>25</sub> H <sub>39</sub> N <sub>2</sub> Cl <sub>6</sub>
0.8812	C <sub>63</sub> H <sub>88</sub> CoN <sub>14</sub> Cl <sub>14</sub> PS•22H <sub>2</sub> O	0.9490	C <sub>74</sub> H <sub>42</sub> Mn <sub>2</sub> N <sub>18</sub> Cl <sub>2</sub> •2C <sub>5</sub> H <sub>5</sub> N
0.8815	C <sub>5</sub> H <sub>5</sub> Cl <sub>2</sub> (N <sub>2</sub> ) <sub>2</sub>	0.9491	C <sub>8</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>2</sub> Cl
0.8820	C <sub>10</sub> H <sub>15</sub> BrCl	0.9504	C <sub>6</sub> H <sub>11</sub> N <sub>3</sub> Cl <sub>4</sub>

P2,2<sub>1</sub>2<sub>1</sub> D<sub>2</sub><sup>4</sup> No. 19 (continued)

## Organic (continued)

0.9512	C <sub>15</sub> H <sub>17</sub> Br <sub>5</sub> •H <sub>2</sub> θ	0.9735	[C <sub>60</sub> H <sub>85</sub> CoN <sub>17</sub> θ <sub>14</sub> P]
0.9519	C <sub>8</sub> H <sub>12</sub> KN <sub>2</sub> θ <sub>3</sub>	0.9743	C <sub>10</sub> H <sub>13</sub> BrN <sub>2</sub> θ <sub>3</sub>
0.9522	C <sub>6</sub> H <sub>3</sub> Br <sub>3</sub>	0.9769	HgClSCN
0.9522	C <sub>16</sub> H <sub>11</sub> Clθ <sub>3</sub>	0.9773	C <sub>21</sub> H <sub>34</sub> θ <sub>5</sub>
0.9554	C <sub>17</sub> H <sub>26</sub> N <sub>8</sub> θ <sub>5</sub> •HBr	0.9790	C <sub>5</sub> H <sub>14</sub> Nθ•Cl
0.9563	C <sub>6</sub> H <sub>5</sub> MgBr•2C <sub>4</sub> H <sub>10</sub> θ	0.9813	[C <sub>59</sub> H <sub>83</sub> CoN <sub>17</sub> θ <sub>14</sub> P]
0.9577	C <sub>18</sub> H <sub>21</sub> θ <sub>3</sub> N	0.9819	[C <sub>15</sub> H <sub>15</sub> ]Brθ <sub>6</sub>
0.9578	C <sub>17</sub> H <sub>20</sub> θ	0.9827	C <sub>21</sub> H <sub>22</sub> N <sub>2</sub> θ <sub>2</sub>
0.9598	C <sub>13</sub> H <sub>7</sub> N <sub>2</sub> Clθ <sub>4</sub>	0.9828	C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> θ <sub>2</sub>
0.9607	C <sub>20</sub> H <sub>14</sub> NiN <sub>2</sub> θ <sub>2</sub>	0.9833	C <sub>10</sub> θH <sub>16</sub> Br <sub>2</sub>
0.9620	C <sub>18</sub> H <sub>21</sub> θ <sub>3</sub> N•H <sub>2</sub> θ	0.9852	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> θ <sub>3</sub> Na
0.9621	C <sub>35</sub> H <sub>41</sub> Nθ <sub>10</sub> •HBr	0.9859	C <sub>14</sub> H <sub>16</sub> θ <sub>5</sub> •H <sub>2</sub> θ
0.9624	C <sub>7</sub> H <sub>5</sub> Brθ <sub>2</sub>	0.9892	C <sub>25</sub> H <sub>37</sub> Nθ <sub>7</sub> •H <sub>2</sub> θ
0.9624	C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> θ•HCl•H <sub>2</sub> θ	0.9906	[(CH <sub>3</sub> ) <sub>4</sub> C <sub>4</sub> C <sub>5</sub> H <sub>5</sub> ]NiC <sub>5</sub> H <sub>5</sub>
0.9626	C <sub>22</sub> H <sub>29</sub> BrN <sub>2</sub> θ <sub>4</sub> •CH <sub>3</sub> θH	0.9919	C <sub>10</sub> H <sub>16</sub> θ:NθH
0.9657	C <sub>6</sub> H <sub>8</sub> θ <sub>4</sub> Se <sub>2</sub>	0.9921	H <sub>2</sub> N•C•(CH <sub>2</sub> θH) <sub>3</sub>
0.9660	C <sub>18</sub> H <sub>12</sub>	0.9925	C <sub>19</sub> H <sub>22</sub> N <sub>2</sub> θ•HBr•H <sub>2</sub> θ
0.9672	[(CH <sub>3</sub> ) <sub>3</sub> NCH <sub>2</sub> CH <sub>2</sub> θH]Cl	0.9928	C <sub>4</sub> H <sub>4</sub> S <sub>3</sub>
0.9689	C <sub>18</sub> H <sub>22</sub> θ <sub>3</sub>	0.9943	(C <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> ) <sub>2</sub> Cθ
0.9713	C <sub>17</sub> H <sub>10</sub> θ	0.9980	C <sub>12</sub> H <sub>9</sub> BrAsN
0.9713	C <sub>8</sub> H <sub>4</sub> θ <sub>12</sub> N <sub>6</sub>	1.0000	C <sub>5</sub> H <sub>3</sub> N(CθθH) <sub>2</sub>
0.9721	CH <sub>3</sub> CCl <sub>2</sub> CH <sub>3</sub>	1.0000	ZnCl <sub>2</sub> •2(C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> θ•HCl)
0.9727	C <sub>12</sub> H <sub>9</sub> AsClN		

2 2 2

C222<sub>1</sub> D<sub>2</sub><sup>5</sup> No. 20Inorganic - 25  
Organic - 34

## Inorganic

0.2357	(Zn, Cu) <sub>5</sub> (Cθ <sub>3</sub> ) <sub>2</sub> (θH) <sub>6</sub>	0.8163	FeFe <sub>4</sub> (θH) <sub>5</sub> (Pθ <sub>4</sub> ) <sub>3</sub>
0.3083	N <sub>2</sub> (Mn, Ca, Sr) <sub>6</sub> Mn <sub>3</sub> (V, As) <sub>6</sub> θ <sub>28</sub> •8H <sub>2</sub> θ	0.8166	Fe <sub>4</sub> Mn(θH) <sub>5</sub> (Pθ <sub>4</sub> ) <sub>3</sub>
0.3913	BaFeF <sub>4</sub>	0.8276	(Fe, Mn)(Fe, Zn) <sub>4</sub> (Pθ <sub>4</sub> ) <sub>3</sub> (θH) <sub>5-2x</sub> •xH <sub>2</sub> θ
0.3952	AlHf	0.8391	Na <sub>2</sub> Tl
0.4014	Ca <sub>5</sub> (θH) <sub>2</sub> (Si <sub>3</sub> θ <sub>8</sub> ) <sub>2</sub> •11H <sub>2</sub> θ	0.8414	(Cu, Fe)Fe <sub>3</sub> (θH) <sub>2</sub> (Pθ <sub>4</sub> ) <sub>3</sub>
0.4125	TaS <sub>3</sub>	0.9055	Mn <sub>2</sub> Pb <sub>2</sub> Si <sub>2</sub> θ <sub>9</sub>
0.4876	Mg <sub>5</sub> (θH) <sub>2</sub> (Cθ <sub>3</sub> ) <sub>4</sub> •4H <sub>2</sub> θ	0.9122	Fe <sub>2</sub> Pb <sub>2</sub> Si <sub>2</sub> θ <sub>9</sub>
0.5000	Ca <sub>5</sub> H <sub>2</sub> (Si <sub>3</sub> θ <sub>9</sub> ) <sub>2</sub> •4H <sub>2</sub> θ	0.9582	K <sub>14</sub> Nb <sub>12</sub> θ <sub>37</sub> •27H <sub>2</sub> θ
0.5338	Na <sub>3</sub> P <sub>3</sub> θ <sub>9</sub> •1.5H <sub>2</sub> θ	0.9756	C <sub>5</sub> Al <sub>6</sub> θ <sub>14</sub>
0.5578	Ca <sub>5</sub> (θH) <sub>2</sub> (Si <sub>3</sub> θ <sub>8</sub> ) <sub>2</sub> •2H <sub>2</sub> θ	0.9978	Pb <sub>2</sub> MgWθ <sub>6</sub>
0.6737	Crθ <sub>3</sub>	1.0000	GaPθ <sub>4</sub>
0.7128	H <sub>2</sub> θ	1.0000	AlPθ <sub>4</sub>
0.8123	(Fe, Mn)Fe <sub>4</sub> (θH) <sub>5</sub> (Pθ <sub>4</sub> ) <sub>3</sub>		

## Organic

0.2357	(Zn, Cu) <sub>5</sub> (Cθ <sub>3</sub> ) <sub>2</sub> (θH) <sub>6</sub>	0.6594	C <sub>2</sub> H <sub>5</sub> •CH:N•NH•C <sub>6</sub> H <sub>3</sub> (Nθ <sub>2</sub> ) <sub>2</sub>
0.4234	Zn[SC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> (NCS) <sub>2</sub>	0.6679	C <sub>19</sub> H <sub>19</sub> Brθ <sub>5</sub>
0.4506	K(Sbθ)C <sub>4</sub> H <sub>4</sub> θ <sub>6</sub> •H <sub>2</sub> θ	0.7011	C <sub>30</sub> H <sub>46</sub> N <sub>6</sub> θ <sub>5</sub> HCl•H <sub>2</sub> θ
0.4657	Rh(Sbθ)C <sub>4</sub> H <sub>4</sub> θ <sub>6</sub> •H <sub>2</sub> θ	0.7546	(C <sub>30</sub> H <sub>46</sub> N <sub>6</sub> θ <sub>5</sub> ) <sub>2</sub> NCCSNH <sub>2</sub>
0.4676	(NH <sub>4</sub> ) <sub>2</sub> Sb <sub>2</sub> (C <sub>4</sub> H <sub>2</sub> θ <sub>6</sub> ) <sub>2</sub> •3H <sub>2</sub> θ	0.7679	C <sub>22</sub> H <sub>34</sub> INθ <sub>5</sub>
0.4730	C <sub>10</sub> H <sub>15</sub> Nθ•0.5H <sub>2</sub> θ	0.7892	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> θ <sub>5</sub> Cl <sub>2</sub>
0.4784	C <sub>6</sub> H <sub>5</sub> θ•C <sub>6</sub> H <sub>7</sub> θ <sub>5</sub> (CθCH <sub>3</sub> ) <sub>4</sub>	0.8099	C <sub>11</sub> H <sub>12</sub> Br <sub>2</sub> N <sub>2</sub> θ <sub>5</sub>
0.4876	Mg <sub>5</sub> (θH) <sub>2</sub> (Cθ <sub>3</sub> ) <sub>4</sub> •4H <sub>2</sub> θ	0.8675	C <sub>28</sub> H <sub>36</sub> •38θ <sub>4</sub>
0.5258	C <sub>15</sub> H <sub>26</sub> N <sub>2</sub> •H <sub>2</sub> θ	0.8900	C <sub>60</sub> H <sub>92</sub> N <sub>12</sub> θ <sub>10</sub> •2HCl•12H <sub>2</sub> θ
0.5353	[C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> θ <sub>4</sub> ] <sub>2</sub> •H <sub>2</sub> Sθ <sub>4</sub> •7H <sub>2</sub> θ	0.9021	C <sub>30</sub> H <sub>46</sub> N <sub>6</sub> θ <sub>5</sub> •H <sub>2</sub> Sθ <sub>4</sub> •xH <sub>2</sub> θ
0.5816	(CH <sub>3</sub> ) <sub>2</sub> Tl(C <sub>5</sub> H <sub>7</sub> θ <sub>2</sub> )	0.9072	C <sub>30</sub> H <sub>46</sub> N <sub>6</sub> θ <sub>5</sub> •HCl•H <sub>2</sub> θ
0.5969	C <sub>6</sub> H <sub>5</sub> ClN <sub>2</sub>	0.9160	C <sub>20</sub> H <sub>13</sub> N
0.5983	Na <sub>4</sub> Zr(C <sub>2</sub> θ <sub>4</sub> ) <sub>4</sub> •3H <sub>2</sub> θ	0.9295	C <sub>30</sub> H <sub>46</sub> N <sub>6</sub> θ <sub>5</sub> •HCl•21H <sub>2</sub> θ
0.5997	Na <sub>4</sub> Hf(C <sub>2</sub> θ <sub>4</sub> ) <sub>4</sub> •3H <sub>2</sub> θ	0.9314	C <sub>30</sub> H <sub>46</sub> N <sub>6</sub> θ <sub>5</sub> HCl•xH <sub>2</sub> θ
0.6338	[N(CH <sub>3</sub> ) <sub>4</sub> ] <sub>2</sub> B <sub>10</sub> H <sub>10</sub> •xH <sub>2</sub> θ	0.9685	C <sub>12</sub> H <sub>8</sub> N <sub>4</sub> KAu
0.6421	C <sub>26</sub> H <sub>33</sub> θ <sub>6</sub> •CθCH <sub>3</sub>	0.9938	C <sub>9</sub> H <sub>11</sub> Ba <sub>2</sub> θ <sub>9</sub> P•8.9H <sub>2</sub> θ
0.6559	C <sub>22</sub> H <sub>28</sub> CoN <sub>2</sub> θ <sub>2</sub>	0.9987	C <sub>28</sub> H <sub>34</sub> N <sub>3</sub> θ <sub>5</sub> Br

2 2 2

C222 D<sub>2</sub><sup>6</sup> No. 21Inorganic - 4  
Organic - 10

## Inorganic

0.2635	AlB <sub>2</sub> Mn <sub>2</sub>	0.5143	Ca <sub>4</sub> NbSi <sub>2</sub> θ <sub>10</sub> (θH, F)
0.3605	U <sub>3</sub> θ <sub>8</sub>	0.7059	Fe <sub>7</sub> Se <sub>8</sub>

C222  $D_2^6$  No. 21 (continued)

## Organic

0.4676	$\text{NiBr}_2 \cdot 2\text{NH}_2\text{C}_6\text{H}_5$	0.6850	$\text{C}_{60}\text{H}_{92}\text{N}_{12}\text{Cl}_{10} \cdot 2\text{HCl} \cdot 10\text{H}_2\text{O}$
0.4723	$\text{CoBr}_2 \cdot 2\text{NH}_2\text{C}_6\text{H}_5$	0.6965	$\text{C}_{30}\text{H}_{46}\text{N}_6\text{Cl}_5 \cdot \text{HCl} \cdot \text{H}_2\text{O}$
0.4755	$\text{NiCl}_2 \cdot 2\text{NH}_2\text{C}_6\text{H}_5$	0.6985	$\text{C}_8\text{H}_{14}\text{N}_4\text{NiCl}_4$
0.4788	$\text{CoCl}_2 \cdot 2\text{NH}_2\text{C}_6\text{H}_5$	0.7284	$\text{C}_{30}\text{H}_{46}\text{N}_6\text{Cl}_5 \cdot \text{H}_2\text{SO}_4 \cdot [x]\text{H}_2\text{O}$
0.4959	$\text{Hg}(\text{SC}_4\text{H}_9)_2$	0.9836	$\text{C}_{22}\text{H}_{28}\text{N}_2\text{Cl}_2\text{Zn}$

2 2 2

F222  $D_2^7$  No. 22Inorganic - 0  
Organic - 1

## Inorganic

.....

## Organic

0.2034  $\text{C}_{20}\text{H}_{13}\text{N}$ 

2 2 2

I222  $D_2^8$  No. 23Inorganic - 1  
Organic - 0

## Inorganic

0.6195  $\text{BPS}_4$ 

## Organic

.....

2 2 2

 $I2_1^2 2_1^2 1^2$   $D_2^9$  No. 24Inorganic - 1  
Organic - 3

## Inorganic

1.0000  $\text{Zr}_2\text{O}_7\text{N}_2$ 

## Organic

0.9703	$\text{C}_{60}\text{H}_{92}\text{N}_{12}\text{Cl}_{10} \cdot 0.55\text{H}_3\text{Hg}_2\text{I}_7 \cdot 0.82\text{HCl} \cdot 2\text{H}_2\text{O}$	0.9781	$\text{C}_{60}\text{H}_{92}\text{N}_{12}\text{Cl}_{10} \cdot 0.65\text{H}_3\text{Hg}_2\text{I}_7 \cdot 0.7\text{HCl} \cdot 14\text{H}_2\text{O}$
0.9777	$\text{C}_{60}\text{H}_{92}\text{N}_{12}\text{Cl}_{10} \cdot 0.65\text{H}_3\text{Hg}_2\text{I}_7 \cdot 0.7\text{HCl} \cdot 2\text{H}_2\text{O}$		

2 m m

m 2 m

m m 2

Pmm2  $C_{2v}^1$  No. 25Inorganic - 8  
Organic - 2

## Inorganic

0.7654	$\text{SiTi}$	0.8654	$\text{Cu}_3\text{Sn}$
0.7660	$\text{GeTi}$	0.9225	$\text{Ag}_3\text{Sb}$
0.7723	$\text{HgNH}_2\text{Cl}$	0.9600	$\text{Al}_2\text{K}(\text{OH}, \text{F})(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$
0.8035	$\text{HgNH}_2\text{Br}$	0.9650	$\text{Bi}_2\text{Ni}_3\text{S}_2$

## Organic

0.5682  $\text{CH}_3 \cdot \text{CH}(\text{OH}) \cdot \text{CH}(\text{NH}_2) \cdot \text{C}_6\text{H}_5$  0.6235  $\text{IiOCCCH}_3 \cdot 2\text{H}_2\text{O}$ 

2 m m

m 2 m

m m 2

Pmc2<sub>1</sub>  $C_{2v}^2$  No. 26Inorganic - 9  
Organic - 4

## Inorganic

0.5139	$\text{Na}_2\text{ZrSi}_6\text{Cl}_{15} \cdot 3\text{H}_2\text{O}$	0.9156	$\text{Ba}(\text{OH})_2 \cdot \text{H}_2\text{O}$
0.5646	$\text{CuGeCl}_3$	0.9232	$\text{Sr}(\text{OH})_2 \cdot \text{H}_2\text{O}$
0.5806	$\text{KF} \cdot 2\text{H}_2\text{O}$	0.9247	$\text{Eu}(\text{OH})_2 \cdot \text{H}_2\text{O}$
0.6354	$\text{Cu}_4(\text{SO}_4)_3(\text{OH})_6 \cdot \text{H}_2\text{O}$	0.9820	$\text{PbO}_x$
0.7072	$\text{Au}_5\text{Zn}_3$		

## Organic

0.5921	$\text{C}_{12}\text{H}_{10}$	0.7400	$\text{C}_6\text{H}_7\text{NCl}$
0.7286	$\text{K}_2\text{C}_2\text{HNCl}_4$	0.7734	$\text{NH}_2\text{C}_6\text{H}_4\text{OH}$

2 m m						
m 2 m		Pcc2	C <sub>2v</sub> <sup>3</sup>	No. 27		Inorganic - 0
m m 2						Organic - 1

Inorganic

.....

Organic

0.9991 K<sub>2</sub>Zr[N(CH<sub>2</sub>COO)<sub>3</sub>]<sub>2</sub>•H<sub>2</sub>O

2 m m						
m 2 m		Pma2	C <sub>2v</sub> <sup>4</sup>	No. 28		Inorganic - 3
m m 2						Organic - 0

Inorganic

0.2962 Ca<sub>2</sub>Al<sub>2</sub>Si<sub>3</sub>O<sub>10</sub>(OH)<sub>2</sub>0.5333 (Au<sub>0.75</sub>Ag<sub>0.25</sub>)Te<sub>2</sub>0.4592 K<sub>2</sub>ZnCl<sub>4</sub>

Organic

.....

2 m m						
m 2 m		Pca2 <sub>1</sub>	C <sub>2v</sub> <sup>5</sup>	No. 29		Inorganic - 9
m m 2						Organic - 44

Inorganic

0.5945 ZnF<sub>2</sub>•4H<sub>2</sub>O0.7072 Cr<sub>3</sub>ClB<sub>7</sub>O<sub>13</sub>0.6007 Na<sub>2</sub>CO<sub>3</sub>•H<sub>2</sub>O0.7075 Mg<sub>3</sub>ClB<sub>7</sub>O<sub>13</sub>

0.6788 GaOCl

0.8745 Fe<sub>2</sub>N0.7000 K<sub>4</sub>XeO<sub>6</sub>•9H<sub>2</sub>O0.9964 KI<sub>2</sub>F<sub>2</sub>0.7069 Fe<sub>3</sub>ClB<sub>7</sub>O<sub>13</sub>

Organic

0.0780 C<sub>36</sub>H<sub>74</sub>0.6183 (NO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>)<sub>3</sub>C0.1450 C<sub>25</sub>H<sub>48</sub>O<sub>5</sub>S<sub>2</sub>0.6324 C<sub>13</sub>H<sub>10</sub>ClNO0.2035 C<sub>17</sub>H<sub>20</sub>N<sub>4</sub>•CH<sub>3</sub>I0.6335 C<sub>10</sub>H<sub>9</sub>NO<sub>3</sub>S0.3147 Co(C<sub>10</sub>H<sub>8</sub>NO<sub>3</sub>S)<sub>2</sub>•9H<sub>2</sub>O0.6662 Cr(O<sub>2</sub>)<sub>2</sub>H<sub>2</sub>O•C<sub>2</sub>H<sub>6</sub>N<sub>2</sub>•H<sub>2</sub>O0.3147 Ni(C<sub>10</sub>H<sub>8</sub>NO<sub>3</sub>S)<sub>2</sub>•9H<sub>2</sub>O0.6737 Ni(C<sub>5</sub>H<sub>7</sub>O<sub>2</sub>)<sub>2</sub>0.3168 Zn(C<sub>10</sub>H<sub>8</sub>NO<sub>3</sub>S)<sub>2</sub>•9H<sub>2</sub>O0.6934 K<sub>2</sub>O•C<sub>6</sub>H<sub>4</sub>•CO<sub>2</sub>H0.3698 (Cl•C<sub>6</sub>H<sub>4</sub>•CO)<sub>2</sub>CH<sub>2</sub>0.7281 (ClCH=CH)<sub>3</sub>SbCl<sub>2</sub>0.4455 CH<sub>2</sub>(NH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>CONHCH<sub>2</sub>CO<sub>2</sub>H•2H<sub>2</sub>O0.7469 K(SbC<sub>4</sub>H<sub>4</sub>O<sub>7</sub>)•0.5H<sub>2</sub>O0.4847 CCl<sub>3</sub>CH(C<sub>6</sub>H<sub>4</sub>I)<sub>2</sub>0.7630 Au(C<sub>3</sub>H<sub>7</sub>)<sub>2</sub>CN0.4978 CCl<sub>3</sub>CH(C<sub>6</sub>H<sub>4</sub>)<sub>2</sub>ClI0.7803 C<sub>13</sub>H<sub>10</sub>I<sub>2</sub>0.5046 CCl<sub>3</sub>CH(C<sub>6</sub>H<sub>4</sub>Br)<sub>2</sub>0.7951 C<sub>11</sub>H<sub>8</sub>O<sub>5</sub>0.5073 C<sub>6</sub>H<sub>2</sub>O<sub>2</sub>(NO<sub>2</sub>)<sub>3</sub>0.8049 C<sub>12</sub>H<sub>19</sub>RhCl<sub>2</sub>•NH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>0.5124 CCl<sub>3</sub>CH(C<sub>6</sub>H<sub>4</sub>)<sub>2</sub>ClBr0.8160 C<sub>6</sub>H<sub>11</sub>NH<sub>2</sub>•HCl0.5175 C<sub>18</sub>H<sub>28</sub>N<sub>4</sub>0.8468 C<sub>6</sub>H<sub>11</sub>NH<sub>2</sub>•HBr0.5204 CCl<sub>3</sub>CH(C<sub>6</sub>H<sub>4</sub>Cl)<sub>2</sub>0.8654 C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O<sub>3</sub>0.5563 C<sub>18</sub>H<sub>18</sub>ClNS0.9002 (CH<sub>3</sub>NH<sub>2</sub>OH)Cl0.5632 C<sub>18</sub>H<sub>18</sub>BrNS0.9181 C<sub>6</sub>H<sub>5</sub>•(C<sub>2</sub>N<sub>2</sub>O)<sub>2</sub>•C<sub>6</sub>H<sub>5</sub>0.5636 C<sub>5</sub>H<sub>5</sub>•Co•C<sub>5</sub>H<sub>5</sub>•C<sub>5</sub>H<sub>4</sub>•C<sub>5</sub>H<sub>5</sub>•Co•C<sub>5</sub>H<sub>5</sub>0.9229 C<sub>12</sub>H<sub>8</sub>Br<sub>2</sub>0.5833 C<sub>17</sub>H<sub>23</sub>N<sub>6</sub>•HBr•H<sub>2</sub>O0.9505 C<sub>4</sub>H<sub>5</sub>S<sub>2</sub>NNH<sub>2</sub>•HCl0.5873 H<sub>4</sub>(H<sub>2</sub>NCSNH<sub>2</sub>)<sub>2</sub>(SCN)<sub>2</sub>0.9583 C<sub>10</sub>H<sub>4</sub>Br<sub>2</sub>O<sub>2</sub>0.5992 (CH<sub>3</sub>)<sub>2</sub>C<sub>4</sub>N<sub>4</sub>Br<sub>2</sub>0.9849 CH<sub>3</sub>NH<sub>3</sub>•Al(SO<sub>4</sub>)<sub>2</sub>•12H<sub>2</sub>O0.6007 Na<sub>2</sub>CO<sub>3</sub>•H<sub>2</sub>O0.9899 Tl<sub>2</sub>CH<sub>3</sub>

2 m m						
m 2 m		Pnc2	C <sub>2v</sub> <sup>6</sup>	No. 30		Inorganic - 3
m m 2						Organic - 8

Inorganic

0.3911 Na<sub>2</sub>S<sub>5</sub>O<sub>6</sub>•2H<sub>2</sub>O0.9354 (Fe, Mn)<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>•3H<sub>2</sub>O0.7750 K<sub>3</sub>Cr(CN)<sub>5</sub>NO

Organic

0.3418 C<sub>27</sub>H<sub>28</sub>0.7307 (NH<sub>4</sub>)<sub>2</sub>HC<sub>6</sub>H<sub>5</sub>O<sub>7</sub>0.4031 C<sub>26</sub>H<sub>26</sub>0.7663 C<sub>10</sub>H<sub>9</sub>NO<sub>3</sub>S0.4193 C<sub>10</sub>H<sub>8</sub>NNaO<sub>3</sub>S•2H<sub>2</sub>O0.7750 K<sub>3</sub>Cr(CN)<sub>5</sub>NO0.4255 Pb(C<sub>10</sub>H<sub>9</sub>O<sub>2</sub>)<sub>2</sub>0.9189 C<sub>10</sub>H<sub>9</sub>NO<sub>3</sub>S

2 m m m 2 m m m 2	Pmn2 <sub>1</sub>	C <sub>2v</sub> <sup>7</sup>	No. 31	Inorganic - 25 Organic - 19
Inorganic				
0.4112	PbB <sub>4</sub> θ <sub>7</sub>		0.6284	NH <sub>4</sub> MgAsθ <sub>4</sub> •6H <sub>2</sub> θ
0.4139	SrB <sub>4</sub> θ <sub>7</sub>		0.7193	CdSθ <sub>4</sub>
0.4229	NaV <sub>2</sub> θ <sub>5</sub>		0.7325	HgSθ <sub>4</sub>
0.4464	WTe <sub>2</sub>		0.7446	Cu(NC <sub>3</sub> ) <sub>2</sub>
0.4725	CuPb <sub>13</sub> Sb <sub>7</sub> S <sub>24</sub>		0.7567	Mn(NC <sub>3</sub> ) <sub>2</sub>
0.5759	Zn(Mnθ <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> θ		0.7730	Te <sub>2</sub> θ <sub>3</sub> Sθ <sub>4</sub>
0.5759	Mg(Mnθ <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> θ		0.8568	Li <sub>3</sub> Pθ <sub>4</sub>
0.5762	Ni(Mnθ <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> θ		0.8639	Cu <sub>3</sub> (As, Sb)S <sub>4</sub>
0.5765	Mg(Clθ <sub>4</sub> ) <sub>2</sub> •6H <sub>2</sub> θ		0.8694	Cu <sub>3</sub> PS <sub>4</sub>
0.6184	MgNH <sub>4</sub> Pθ <sub>4</sub> •6H <sub>2</sub> θ		0.8694	Cu <sub>3</sub> AsS <sub>4</sub>
0.6193	MgNH <sub>4</sub> Asθ <sub>4</sub> •6H <sub>2</sub> θ		0.9239	AsCuPbS <sub>3</sub>
0.6196	MgNH <sub>4</sub> Pθ <sub>4</sub> •6H <sub>2</sub> θ		0.9370	CuPbSbS <sub>3</sub>
0.6216	MgNH <sub>4</sub> Pθ <sub>4</sub> •6H <sub>2</sub> θ			
Organic				
0.2808	C <sub>22</sub> H <sub>35</sub> IN <sub>2</sub> θ <sub>2</sub>		0.8037	Ga(CH <sub>2</sub> CθCH <sub>2</sub> CθCH <sub>3</sub> ) <sub>3</sub>
0.3555	C <sub>4</sub> H <sub>9</sub> HgCl		0.8121	In(CH <sub>2</sub> CθCH <sub>2</sub> CθCH <sub>3</sub> ) <sub>3</sub>
0.4487	[Co(NH <sub>3</sub> ) <sub>4</sub> Cθ <sub>3</sub> ]Clθ <sub>4</sub>		0.8193	B <sub>9</sub> C <sub>2</sub> H <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub>
0.4958	Cd[SC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> Cl <sub>2</sub>		0.8372	Sc(CH <sub>2</sub> CθCH <sub>2</sub> CθCH <sub>3</sub> ) <sub>3</sub>
0.5168	[(CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ] <sub>2</sub> SnCl <sub>6</sub>		0.8794	C <sub>24</sub> H <sub>16</sub> P <sub>3</sub>
0.5727	B <sub>4</sub> H <sub>6</sub> C <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub>		0.9098	C <sub>3</sub> H <sub>6</sub> Se <sub>3</sub>
0.7130	K <sub>3</sub> Mo(NCS) <sub>6</sub> •H <sub>2</sub> θ•CH <sub>3</sub> CθθR		0.9102	(CH <sub>3</sub> ) <sub>3</sub> GeCN
0.7556	Cu(C <sub>8</sub> H <sub>14</sub> N <sub>6</sub> θS <sub>2</sub> )		0.9132	C <sub>3</sub> H <sub>6</sub> S <sub>3</sub>
0.7909	C <sub>14</sub> H <sub>28</sub> NI		0.9954	C <sub>10</sub> H <sub>20</sub> IN
0.7930	C <sub>4</sub> H <sub>8</sub> θ <sub>2</sub> S <sub>2</sub>			
2 m m m 2 m m m 2	Pba2	C <sub>2v</sub> <sup>8</sup>	No. 32	Inorganic - 5 Organic - 2
Inorganic				
0.3015	Rb <sub>3</sub> Sb <sub>5</sub> θ <sub>14</sub>		0.6984	PbZrθ <sub>3</sub>
0.3024	K <sub>3</sub> Sb <sub>5</sub> θ <sub>14</sub>		0.9082	Mo <sub>17</sub> θ <sub>47</sub>
0.6641	Al <sub>18</sub> Si <sub>6</sub> θ <sub>39</sub>			
Organic				
0.6244	CCl <sub>3</sub> •CH(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>		0.6336	[Co(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> Cl <sub>2</sub> ] <sub>2</sub> •S <sub>6</sub> θ <sub>6</sub> •H <sub>2</sub> θ
2 m m m 2 m m m 2	Pna2 <sub>1</sub>	C <sub>2v</sub> <sup>9</sup>	No. 33	Inorganic - 55 Organic - 100
Inorganic				
0.4161	Na <sub>2</sub> Si <sub>2</sub> θ <sub>5</sub>		0.5575	NaYSiθ <sub>4</sub>
0.4282	Cr(NH <sub>3</sub> ) <sub>3</sub> θ <sub>4</sub>		0.6025	H <sub>3</sub> Pθ <sub>3</sub>
0.4345	PbZnSiθ <sub>4</sub>		0.6967	Pb(N <sub>3</sub> ) <sub>2</sub>
0.4612	Sb <sub>2</sub> θ <sub>4</sub>		0.7113	NaTaθ <sub>3</sub>
0.4629	Sb <sub>2</sub> θ <sub>4</sub>		0.7114	CdTlθ <sub>3</sub>
0.4685	SbTaθ <sub>4</sub>		0.7261	HNθ <sub>3</sub> •H <sub>2</sub> θ
0.4692	SbTaθ <sub>4</sub>		0.7417	K <sub>2</sub> BeF <sub>4</sub>
0.4705	SbNbθ <sub>4</sub>		0.7599	NaAlθ <sub>2</sub>
0.4705	SbTaθ <sub>4</sub>		0.7784	Tb(Reθ <sub>4</sub> ) <sub>3</sub> •4H <sub>2</sub> θ
0.4708	SbNbθ <sub>4</sub>		0.7792	Sb <sub>2</sub> Yb <sub>5</sub>
0.4712	SbNbθ <sub>4</sub>		0.7814	Nd(Reθ <sub>4</sub> ) <sub>3</sub> •4H <sub>2</sub> θ
0.4733	PbCN <sub>2</sub>		0.7948	NaFeθ <sub>2</sub>
0.4789	BiTaθ <sub>4</sub>		0.8233	BaHPθ <sub>4</sub>
0.4807	CuAsS		0.8402	[RuNθ(NH <sub>3</sub> ) <sub>5</sub> ]Cl <sub>3</sub> •H <sub>2</sub> θ
0.4847	BiNbθ <sub>4</sub>		0.8412	BaBe <sub>2</sub> Si <sub>2</sub> θ <sub>7</sub>
0.5003	Zn(N <sub>3</sub> ) <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub>		0.8419	SbSI
0.5176	CaB <sub>3</sub> θ <sub>5</sub> (θH)		0.8478	LiGaθ <sub>2</sub>
0.5231	Ge <sub>4</sub> Y <sub>5</sub>		0.8627	Li <sub>3</sub> AlF <sub>6</sub>
0.5247	Sm <sub>5</sub> Ge <sub>4</sub>		0.8634	BaSiθ <sub>3</sub> •6H <sub>2</sub> θ
0.5261	Si <sub>4</sub> Y <sub>5</sub>		0.8726	(Sθ <sub>3</sub> ) <sub>3</sub>
0.5261	Gd <sub>5</sub> Ge <sub>4</sub>		0.9044	Li(N <sub>2</sub> H <sub>5</sub> ) <sub>5</sub> θ <sub>4</sub>
0.5265	Ge <sub>4</sub> Nd <sub>5</sub>		0.9098	LiV <sub>2</sub> θ <sub>5</sub>
0.5266	Ge <sub>4</sub> Tb <sub>5</sub>		0.9297	FeAlθ <sub>3</sub>
0.5267	Er <sub>5</sub> Ge <sub>4</sub>		0.9310	GaFeθ <sub>3</sub>
0.5274	Si <sub>4</sub> Tb <sub>5</sub>		0.9525	Zn(Nθ <sub>3</sub> ) <sub>2</sub> •6H <sub>2</sub> θ
0.5293	Er <sub>5</sub> Si <sub>4</sub>		0.9811	MgSθ <sub>3</sub> •3H <sub>2</sub> θ
0.5314	Cu <sub>3</sub> Mo <sub>2</sub> θ <sub>9</sub>		0.9950	NH <sub>4</sub> I•3NH <sub>3</sub>
0.5510	Na <sub>2</sub> BeF <sub>4</sub>			

Pna2<sub>1</sub> C<sub>2v</sub><sup>9</sup> No. 33 (continued)

## Organic

0.2293	C <sub>8</sub> H <sub>7</sub> Br <sub>2</sub>	0.6498	C <sub>20</sub> H <sub>32</sub> As <sub>4</sub> AuI
0.2500	C <sub>10</sub> H <sub>8</sub> KN <sub>2</sub> O <sub>3</sub> S	0.6554	(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> Ni <sub>2</sub> C <sub>6</sub> H <sub>5</sub> •C•C <sub>6</sub> H <sub>5</sub>
0.2559	C <sub>6</sub> H <sub>4</sub> N <sub>4</sub>	0.6596	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>
0.2751	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> Br	0.6676	Cl(N <sub>2</sub> )C <sub>6</sub> H <sub>3</sub> NH <sub>2</sub>
0.2804	Cl•C <sub>6</sub> H <sub>4</sub> N <sub>2</sub>	0.6680	C <sub>6</sub> H <sub>7</sub> N <sub>5</sub> •2HBr
0.3070	NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> •C <sub>6</sub> H <sub>4</sub> Br	0.6721	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> •HCHBrCl <sub>2</sub>
0.3132	NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> •C <sub>6</sub> H <sub>4</sub> Cl	0.6877	H <sub>3</sub> BC <sub>6</sub> •2CH <sub>3</sub> NH <sub>2</sub>
0.3364	(C <sub>6</sub> H <sub>4</sub> CH=N(CH <sub>2</sub> ) <sub>2</sub> N•CHC <sub>6</sub> H <sub>4</sub> •)Zn•H <sub>2</sub> •	0.7073	C <sub>10</sub> H <sub>16</sub> Cl <sub>2</sub> Pt
0.3399	C <sub>6</sub> H <sub>5</sub> •C <sub>4</sub> H <sub>7</sub> S <sub>2</sub>	0.7094	C <sub>9</sub> H <sub>10</sub> BrN <sub>2</sub>
0.3547	C <sub>6</sub> (N <sub>2</sub> ) <sub>6</sub>	0.7106	Na[Co(C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ]•4H <sub>2</sub> •
0.3713	ErC <sub>2</sub> ClH <sub>2</sub> Hg	0.7118	C <sub>10</sub> H <sub>3</sub> Br <sub>3</sub> •
0.3739	C <sub>12</sub> H <sub>9</sub> N <sub>2</sub> SCL	0.7287	C <sub>6</sub> H <sub>6</sub> Br <sub>2</sub>
0.3883	C <sub>20</sub> H <sub>13</sub> NSe	0.7331	C <sub>4</sub> H <sub>3</sub> BrN <sub>2</sub> •
0.4083	C <sub>20</sub> H <sub>16</sub>	0.7492	C <sub>3</sub> H <sub>15</sub> N <sub>11</sub> Ni <sub>6</sub> S <sub>3</sub> •H <sub>2</sub> •
0.4132	[(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> AsC <sub>6</sub> H <sub>4</sub> ] <sub>3</sub> As•RuBr <sub>2</sub>	0.7533	C <sub>18</sub> H <sub>15</sub> SeCl
0.4135	C <sub>21</sub> H <sub>13</sub> N	0.7554	ClC <sub>6</sub> H <sub>4</sub> NHC <sub>6</sub> H <sub>3</sub>
0.4332	CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub>	0.7554	LiI•5(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> P <sub>6</sub>
0.4512	(C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> •)FeCl•CH <sub>3</sub> N <sub>2</sub>	0.7584	C <sub>8</sub> H <sub>6</sub> I <sub>2</sub>
0.4733	PbCN <sub>2</sub>	0.7706	C <sub>3</sub> H <sub>5</sub> PdC <sub>5</sub> H <sub>5</sub>
0.4770	Fe(CH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>3</sub> ) <sub>3</sub>	0.7785	C <sub>6</sub> H <sub>4</sub> •HBrN <sub>2</sub>
0.4793	Al(CH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>3</sub> ) <sub>3</sub>	0.7837	H <sub>2</sub> C•CHNH <sub>2</sub> •C <sub>6</sub> H <sub>5</sub>
0.4795	Ga(CH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>3</sub> ) <sub>3</sub>	0.7891	C <sub>6</sub> H <sub>4</sub> •HN <sub>2</sub> Cl
0.4796	S(CH <sub>2</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.7920	[(CH <sub>3</sub> ) <sub>3</sub> S] <sub>2</sub> HgI <sub>4</sub>
0.4956	C <sub>9</sub> H <sub>18</sub> NI	0.8057	(CH <sub>3</sub> ) <sub>2</sub> •C•P(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •NH <sub>2</sub> •H <sub>2</sub> •
0.4982	C <sub>18</sub> H <sub>12</sub>	0.8115	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>
0.5017	CH <sub>3</sub> CH(NH <sub>2</sub> )C <sub>6</sub> H <sub>5</sub>	0.8135	C <sub>9</sub> H <sub>7</sub> N <sub>2</sub> •HgCl <sub>2</sub>
0.5077	Se(CH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>3</sub> ) <sub>3</sub>	0.8271	C <sub>6</sub> H <sub>9</sub> •PS
0.5125	In(CH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>3</sub> ) <sub>3</sub>	0.8438	C <sub>6</sub> H <sub>4</sub> •NH <sub>2</sub> •C <sub>6</sub> H <sub>5</sub>
0.5227	C <sub>4</sub> H <sub>6</sub> Br <sub>2</sub> S <sub>2</sub>	0.8629	C <sub>8</sub> H <sub>6</sub> N <sub>3</sub> I
0.5364	MnCl <sub>2</sub> •2(CH <sub>2</sub> ) <sub>6</sub> N <sub>4</sub> •2H <sub>2</sub> •	0.8687	C <sub>33</sub> H <sub>36</sub> •
0.5412	Ni(SC <sub>2</sub> H <sub>4</sub> N=C(CH <sub>3</sub> )C(CH <sub>3</sub> )=NC <sub>2</sub> H <sub>4</sub> S)	0.8805	Ni(C <sub>5</sub> H <sub>5</sub> N) <sub>4</sub> Br <sub>2</sub>
0.5423	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> S•H <sub>2</sub> •	0.8868	C <sub>4</sub> H <sub>8</sub> S <sub>2</sub>
0.5500	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> SI	0.8931	Co(C <sub>5</sub> H <sub>5</sub> N) <sub>4</sub> Br <sub>2</sub>
0.5555	C <sub>9</sub> H <sub>11</sub> •N	0.8983	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> •S <sub>2</sub>
0.5670	Pb[SC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> Cl <sub>2</sub>	0.9017	B <sub>10</sub> Br <sub>2</sub> H <sub>8</sub> C <sub>2</sub> H <sub>2</sub>
0.5692	C <sub>24</sub> H <sub>18</sub>	0.9050	C <sub>6</sub> H <sub>6</sub> •
0.5719	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> CH	0.9155	C <sub>10</sub> H <sub>9</sub> N <sub>2</sub> S
0.5733	(C <sub>5</sub> H <sub>5</sub> )Fe(C <sub>5</sub> H <sub>4</sub> •C <sub>6</sub> H <sub>3</sub> (•H) <sub>2</sub> )	0.9260	C <sub>10</sub> H <sub>9</sub> N
0.5830	C <sub>9</sub> H <sub>18</sub> N <sub>4</sub> •3HCl•0.5H <sub>2</sub> •	0.9292	Cr(C <sub>6</sub> ) <sub>6</sub>
0.5870	Pb(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub>	0.9343	Mo(C <sub>6</sub> ) <sub>6</sub>
0.5990	Be(C <sub>2</sub> H <sub>4</sub> ) <sub>3</sub> •3H <sub>2</sub> •	0.9397	Pt[(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> P] <sub>2</sub> HBr
0.6027	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub>	0.9437	C <sub>6</sub> H <sub>4</sub> (N <sub>2</sub> ) <sub>2</sub>
0.6072	C <sub>19</sub> H <sub>12</sub> •	0.9471	W(C <sub>6</sub> ) <sub>6</sub>
0.6279	[(H <sub>4</sub> C <sub>6</sub> P(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> As(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ] <sub>2</sub> Cu)I	0.9488	C <sub>9</sub> H <sub>8</sub> BrN <sub>2</sub>
0.6290	C <sub>3</sub> H <sub>7</sub> •NH <sub>2</sub> •C <sub>4</sub> H <sub>9</sub> Cl	0.9643	C <sub>6</sub> H <sub>4</sub> SN <sub>2</sub>
0.6293	C <sub>6</sub> H <sub>4</sub> (•H) <sub>2</sub>	0.9743	Br(CH <sub>3</sub> )C <sub>6</sub> H <sub>3</sub> •H
0.6313	[(H <sub>4</sub> C <sub>6</sub> P(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> As(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ] <sub>2</sub> Au)I	0.9783	C <sub>10</sub> H <sub>8</sub> •
0.6343	C <sub>15</sub> H <sub>11</sub> Cl <sub>4</sub> S <sub>2</sub>	0.9817	Co(NH <sub>3</sub> ) <sub>5</sub> C <sub>6</sub> H <sub>3</sub> Br•H <sub>2</sub> •
0.6349	C <sub>6</sub> H <sub>7</sub> N <sub>2</sub>	0.9888	C <sub>7</sub> H <sub>5</sub> Cl <sub>2</sub>
0.6428	U <sub>2</sub> (CH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> •2H <sub>2</sub> •	0.9912	C <sub>6</sub> H <sub>4</sub> SeN <sub>2</sub>

2 m m  
m 2 m  
m m 2Pnn2 C<sub>2v</sub><sup>10</sup> No. 34Inorganic - 6  
Organic - 0

## Inorganic

0.9766	Ca <sub>2</sub> NaAl <sub>5</sub> Si <sub>5</sub> •20•6H <sub>2</sub> •	0.9856	Ca <sub>8</sub> (Ti, Na) <sub>4</sub> Al <sub>20</sub> Si <sub>20</sub> •80•20H <sub>2</sub> •
0.9841	Ca <sub>8</sub> (Ag, Na) <sub>4</sub> Al <sub>20</sub> Si <sub>20</sub> •80•18H <sub>2</sub> •	0.9879	Ca <sub>2</sub> NaAl <sub>5</sub> Si <sub>5</sub> •20•6H <sub>2</sub> •
0.9848	Ca <sub>2</sub> NaAl <sub>5</sub> Si <sub>5</sub> •20•6H <sub>2</sub> •	0.9894	NaCa <sub>2</sub> Al <sub>5</sub> Si <sub>5</sub> •20•6H <sub>2</sub> •

## Organic

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2 m m  
m 2 m  
m m 2Cmm2 C<sub>2v</sub><sup>11</sup> No. 35Inorganic - 4  
Organic - 2

## Inorganic

0.9867	Cd(NH <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	1.0000	Hg(NH <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>
1.0000	Cd(NH <sub>3</sub> ) <sub>2</sub> Br <sub>2</sub>	1.0000	Mg <sub>3</sub> ClB <sub>7</sub> •13

Cmm2  $C_{2v}^{11}$  No. 35 (continued)

Organic  
 0.5970  $CH_3C\theta\theta Li \cdot 2H_2\theta$  0.9520  $Te(C_3H_6N_2S)_4 TeCl_6$

2 m m  
 m 2 m  
 m m 2

Cmc2<sub>1</sub>  $C_{2v}^{12}$  No. 36

Inorganic - 29  
 Organic - 9

Inorganic  
 0.4051 AgCa 0.6315  $Rb_2UF_6$   
 0.4456 MoP<sub>2</sub> 0.6664  $K_2Pb\theta_3$   
 0.4456 P<sub>2</sub>W 0.6883  $As_5SbS_4$   
 0.5073  $(Ag_4Te)(N\theta_3)_2$  0.6908  $K_2\theta_8NCl_5$   
 0.5144 Sn $\theta$  0.6932  $K_2\theta_8NCl_5$   
 0.5320 HgI<sub>2</sub> 0.7132  $K\theta_8NBr_4 \cdot 2H_2\theta$   
 0.5462 HgBr<sub>2</sub> 0.8500  $Al_{22.95}Cu_{1.05}Fe_4$   
 0.5549  $Pb_{18}Sb_{18}S_{44}$  0.8703  $U\theta_2(N\theta_3)_2 \cdot 6H_2\theta$   
 0.5708  $Be_2(Be\theta H)_2Si\theta_3Si\theta_4$  0.8836  $Ni_3Si_2$   
 0.5722  $Na_2Ge\theta_3$  0.8992 BrF<sub>3</sub>  
 0.5764  $Li_2Si\theta_3$  0.9209  $B_6H_{10}$   
 0.5772  $Na_2Si\theta_3$  0.9234 BrF<sub>5</sub>  
 0.5774  $Li_2Ge\theta_3$  0.9360  $Al_4\theta_4C$   
 0.6189  $Si_2N_2\theta$  0.9497  $NbI_4$   
 0.6253  $Rb_2AmF_6$

Organic  
 0.4116  $C_6H_4I_2$  0.6518  $C_7H_7N\theta \cdot HCl$   
 0.5229  $C_4D_3N_3\theta_4 \cdot D_2\theta$  0.6525  $C_4H_4S_2$   
 0.5229  $C_4H_3N_3\theta_4 \cdot H_2\theta$  0.8634  $CH_3Cl$   
 0.5735  $C_7H_8 \cdot 2AgN\theta_3$  0.9360  $Al_4\theta_4C$   
 0.6028  $ErCH(CH\theta)_2$

2 m m  
 m 2 m  
 m m 2

Ccc2  $C_{2v}^{13}$  No. 37

Inorganic - 0  
 Organic - 4

Inorganic

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Organic  
 0.2772  $(BrC_6H_4)_2S_2$  0.4033  $C_9H_9K\theta_4 \cdot 2H_2\theta$   
 0.2792  $(BrC_6H_4)_2C\theta$  0.8070  $C_{14}H_{14}N_2\theta_2$

2 m m  
 m 2 m  
 m m 2

Amm2  $C_{2v}^{14}$  No. 38

Inorganic - 7  
 Organic - 2

Inorganic  
 0.4266  $CsH_2P\theta_4$  0.6472  $Na_2Ca_2(C\theta_3)_3$   
 0.5613  $U_3\theta_8$  0.6904  $NaNb_6\theta_{15}(\theta H)$   
 0.6007  $U\theta_3$  0.6923  $NaNb_6\theta_{15}F$   
 0.6455  $Na_2Ca_2(C\theta_3)_3$

Organic  
 0.6455  $Na_2Ca_2(C\theta_3)_3$  0.6472  $Na_2Ca_2(C\theta_3)_3$

2 m m  
 m 2 m  
 m m 2

Abm2  $C_{2v}^{15}$  No. 39

Inorganic - 2  
 Organic - 5

Inorganic  
 0.4916  $Cu_2S$  0.5731  $La_2(S\theta_4)_3 \cdot 8H_2\theta$

Organic  
 0.1893  $(IC_6H_4CH:)_2C_5H_4\theta$  0.9527  $C_7H_{15}N \cdot HBr$   
 0.1942  $BrC_6H_4 \cdot CH \cdot C_5H_4\theta \cdot CH \cdot C_6H_5Br$  0.9664  $C_7H_{15}N \cdot HI$   
 0.8387  $Fe(C_5H_4C\theta C_3H_7)_2$

2 m m									
m 2 m		Ama2	C <sub>2v</sub> <sup>16</sup>	No. 40				Inorganic - 9	
m m 2								Organic - 2	
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Inorganic									
0.3804	DyGe			0.9680	SbF <sub>3</sub>				
0.3935	GdGe			0.9957	Cs <sub>3</sub> Re <sub>3</sub> Cl <sub>12</sub>				
0.3939	GaGd			1.0000	(K <sub>x</sub> Na <sub>1-x</sub> )Si <sub>11</sub> Al <sub>5</sub> Cl <sub>32</sub> •10H <sub>2</sub> O				
0.5785	Pt <sub>2</sub> U			1.0000	Cs <sub>3</sub> Re <sub>3</sub> Br <sub>12</sub>				
0.6711	CrCl <sub>3</sub>								
-----									
Organic									
0.6852	(C <sub>2</sub> N <sub>2</sub> H <sub>8</sub> )PtBr <sub>3</sub>			0.7711	C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> S				
-----									
2 m m									
m 2 m		Aba2	C <sub>2v</sub> <sup>17</sup>	No. 41				Inorganic - 15	
m m 2								Organic - 14	
-----									
Inorganic									
0.5252	CoGe <sub>2</sub>			0.7747	Al(Fe, Mn)(OH) <sub>2</sub> Pd <sub>4</sub> •H <sub>2</sub> O				
0.5281	RhSn <sub>2</sub>			0.7759	AlFe(OH) <sub>2</sub> Pd <sub>4</sub> •H <sub>2</sub> O				
0.5329	PdSn <sub>2</sub>			0.9544	Ca <sub>2</sub> UCl <sub>2</sub> (C <sub>6</sub> H <sub>3</sub> ) <sub>3</sub> •10-11H <sub>2</sub> O				
0.5587	PdSn <sub>4</sub>			0.9740	NH <sub>4</sub> B <sub>5</sub> Cl <sub>8</sub> •4H <sub>2</sub> O				
0.5592	AuSn <sub>4</sub>			0.9899	K[B <sub>5</sub> Cl <sub>6</sub> (OH) <sub>4</sub> ]•2H <sub>2</sub> O				
0.5658	PtSn <sub>4</sub>			0.9905	KH <sub>2</sub> (B <sub>3</sub> Cl) <sub>2</sub> B <sub>5</sub> Cl <sub>10</sub>				
0.7435	Hf <sub>7</sub> Ni <sub>10</sub>			0.9986	S <sub>2</sub>				
0.7437	Ni <sub>10</sub> Zr <sub>7</sub>								
-----									
Organic									
0.2735	(CH <sub>3</sub> ClC <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> N <sub>2</sub>			0.3498	C <sub>18</sub> H <sub>16</sub>				
0.2851	C <sub>22</sub> H <sub>14</sub>			0.3524	C <sub>6</sub> H <sub>4</sub> (C <sub>6</sub> H <sub>5</sub> )(C <sub>6</sub> H <sub>5</sub> Na)				
0.2908	C <sub>22</sub> H <sub>14</sub>			0.3553	C <sub>17</sub> H <sub>14</sub>				
0.2948	C <sub>21</sub> H <sub>14</sub>			0.3798	C <sub>16</sub> H <sub>14</sub>				
0.3199	C <sub>22</sub> H <sub>18</sub>			0.7722	C <sub>6</sub> H <sub>5</sub> •C <sub>7</sub> H <sub>4</sub> N <sub>2</sub>				
0.3238	C <sub>17</sub> H <sub>16</sub>			0.8596	Ni(C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> Cl <sub>2</sub> ) <sub>2</sub> •2H <sub>2</sub> O				
0.3460	C <sub>16</sub> H <sub>14</sub>			0.9544	Ca <sub>2</sub> UCl <sub>2</sub> (C <sub>6</sub> H <sub>3</sub> ) <sub>3</sub> •10-11H <sub>2</sub> O				
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2 m m									
m 2 m		Fmm2	C <sub>2v</sub> <sup>18</sup>	No. 42				Inorganic - 0	
m m 2								Organic - 0	
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.....									
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2 m m									
m 2 m		Fdd2	C <sub>2v</sub> <sup>19</sup>	No. 43				Inorganic - 25	
m m 2								Organic - 25	
-----									
Inorganic									
0.4239	Cd(NCl <sub>3</sub> ) <sub>2</sub> •4H <sub>2</sub> O			0.9374	Li <sub>2</sub> Al <sub>2</sub> Si <sub>3</sub> Cl <sub>10</sub> •2H <sub>2</sub> O				
0.4254	Cd(NCl <sub>3</sub> ) <sub>2</sub> •4H <sub>2</sub> O			0.9573	SnI <sub>4</sub> •2S <sub>8</sub>				
0.4889	Th(NCl <sub>3</sub> ) <sub>4</sub> •5H <sub>2</sub> O			0.9677	Li <sub>2</sub> Al <sub>2</sub> Si <sub>3</sub> Cl <sub>10</sub> •2H <sub>2</sub> O				
0.4925	Ce(NCl <sub>3</sub> ) <sub>4</sub> •5H <sub>2</sub> O			0.9728	(NH <sub>4</sub> ) <sub>2</sub> Al <sub>2</sub> Si <sub>3</sub> Cl <sub>10</sub>				
0.4934	Fu(NCl <sub>3</sub> ) <sub>4</sub> •5H <sub>2</sub> O			0.9769	Na <sub>2</sub> Al <sub>2</sub> Si <sub>3</sub> Cl <sub>10</sub> •2H <sub>2</sub> O				
0.4982	P <sub>2</sub> S <sub>5</sub>			0.9812	Na <sub>2</sub> Al <sub>2</sub> Si <sub>3</sub> Cl <sub>10</sub> •2H <sub>2</sub> O				
0.5219	GeS <sub>2</sub>			0.9832	Na <sub>2</sub> Al <sub>2</sub> Si <sub>3</sub> Cl <sub>10</sub> •2H <sub>2</sub> O				
0.5424	S <sub>2</sub> (NH <sub>2</sub> ) <sub>2</sub>			0.9839	Na <sub>2</sub> Al <sub>2</sub> Si <sub>3</sub> Cl <sub>10</sub> •2H <sub>2</sub> O				
0.5643	CaNa <sub>2</sub> (C <sub>6</sub> H <sub>3</sub> ) <sub>2</sub> •2H <sub>2</sub> O			0.9841	Ag <sub>2</sub> Al <sub>2</sub> Si <sub>3</sub> Cl <sub>10</sub> •2H <sub>2</sub> O				
0.5669	CaSiCl <sub>3</sub> •H <sub>2</sub> O			0.9865	Ca <sub>2</sub> Na <sub>2</sub> (Al <sub>2</sub> Si <sub>3</sub> Cl <sub>10</sub> ) <sub>3</sub> •8H <sub>2</sub> O				
0.5716	N <sub>2</sub> H <sub>5</sub> Cl			0.9915	KB <sub>2</sub> F <sub>4</sub>				
0.6904	Al <sub>3</sub> Zr <sub>2</sub>			1.0000	Na <sub>2</sub> BeSi <sub>2</sub> Cl <sub>6</sub>				
0.6919	Al <sub>3</sub> Hf <sub>2</sub>								
-----									
Organic									
0.2541	C <sub>15</sub> H <sub>24</sub> ClNCl			0.7097	C <sub>5</sub> H <sub>5</sub> Rh(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub>				
0.4003	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> Ti <sub>2</sub>			0.7186	Ni(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> NCl <sub>2</sub> Cl				
0.4066	CoI <sub>2</sub> •2NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>3</sub>			0.7210	Ni(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> NCl <sub>2</sub> Br				
0.4852	CH <sub>2</sub> (N <sub>2</sub> Cl <sub>2</sub> K) <sub>2</sub>			0.7297	NCl <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> •N:NBF <sub>4</sub>				
0.5002	C <sub>6</sub> H <sub>8</sub> Br <sub>4</sub>			0.7738	C <sub>9</sub> H <sub>12</sub> Cl <sub>4</sub> S <sub>3</sub>				
0.5027	C <sub>12</sub> H <sub>8</sub> Cl <sub>2</sub> S <sub>2</sub>			0.7821	([C <sub>6</sub> H <sub>5</sub> ] <sub>3</sub> AsCH <sub>3</sub> ) <sub>2</sub> CuCl <sub>4</sub>				
0.5097	(C <sub>6</sub> H <sub>5</sub> •CH:CH•CH <sub>2</sub> •S-) <sub>2</sub>			0.7927	NCl <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> •N:N•PF <sub>6</sub>				
0.5478	KLa[(ClCCl <sub>2</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(CH <sub>2</sub> Cl) <sub>2</sub> ]•8H <sub>2</sub> O			0.8087	C <sub>10</sub> H <sub>20</sub> Cl <sub>2</sub> •H <sub>2</sub> O				
0.5495	(BrHg) <sub>2</sub> Fe(C <sub>6</sub> H <sub>4</sub> ) <sub>4</sub>			0.8460	Ca(UCl <sub>2</sub> ) <sub>2</sub> (CH <sub>3</sub> CO <sub>2</sub> ) <sub>6</sub> •6H <sub>2</sub> O				
0.5643	CaNa <sub>2</sub> (C <sub>6</sub> H <sub>3</sub> ) <sub>2</sub> •2H <sub>2</sub> O			0.9073	C <sub>20</sub> H <sub>12</sub> N <sub>2</sub> Cl <sub>2</sub>				
0.6337	C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> Cl <sub>8</sub>			0.9725	Hg(C <sub>13</sub> H <sub>11</sub> N <sub>4</sub> S) <sub>2</sub> •2C <sub>5</sub> H <sub>5</sub> N				
0.6350	ZnH <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> ) <sub>4</sub> •2H <sub>2</sub> O			0.9914	[(NH <sub>2</sub> ) <sub>2</sub> CS] <sub>2</sub> Te(SCN) <sub>2</sub>				
0.7083	CH <sub>4</sub> N <sub>4</sub> Cl <sub>2</sub>								



2 m m m 2 m m m 2	Imm2	C <sub>2v</sub> <sup>20</sup>	No. 44	Inorganic - 10 Organic - 4
Inorganic				
0.4588	Sn <sub>5</sub> Ti <sub>6</sub>		0.7832	Zn <sub>4</sub> (OH) <sub>2</sub> Si <sub>2</sub> O <sub>7</sub> •H <sub>2</sub> O
0.7229	Cd <sub>2</sub> Sb <sub>2</sub> O <sub>7</sub>		0.8344	KCN
0.7308	Ca <sub>2</sub> Sb <sub>2</sub> O <sub>7</sub>		0.8404	AgNO <sub>2</sub>
0.7317	Na <sub>2</sub> MgAlF <sub>7</sub>		0.8948	HCN
0.7809	Zn <sub>4</sub> (OH) <sub>2</sub> Si <sub>2</sub> O <sub>7</sub> •H <sub>2</sub> O		0.9676	NaN <sub>2</sub>
Organic				
0.5778	C <sub>7</sub> H <sub>6</sub> ClN <sub>2</sub>		0.8344	KCN
0.8120	[(CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> ] <sub>2</sub> SbCl <sub>6</sub>		0.8948	HCN
2 m m m 2 m m m 2	Iba2	C <sub>2v</sub> <sup>21</sup>	No. 45	Inorganic - 0 Organic - 11
Inorganic				
.....				
Organic				
0.1548	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> COCCONa		0.5105	(CH <sub>3</sub> ) <sub>3</sub> CC(CH <sub>3</sub> )(OH)CH=CH <sub>2</sub> •0.5H <sub>2</sub> O
0.4906	CH <sub>3</sub> •COH(CH <sub>3</sub> )•CCl <sub>3</sub> •0.5H <sub>2</sub> O		0.8497	C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>
0.4925	C(CH <sub>3</sub> ) <sub>3</sub> COH(CH <sub>3</sub> )CH <sub>3</sub> •0.5H <sub>2</sub> O		0.8709	(BrC <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> SeCl <sub>2</sub>
0.4972	C <sub>8</sub> H <sub>16</sub> O•0.5H <sub>2</sub> O		0.8731	(BrC <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> SeBr <sub>2</sub>
0.5044	C <sub>2</sub> (CH <sub>3</sub> ) <sub>5</sub> OH		0.9339	C <sub>3</sub> H <sub>7</sub> •C <sub>12</sub> H <sub>8</sub> N
0.5093	(CH <sub>3</sub> ) <sub>3</sub> CC(CH <sub>3</sub> )(OH)C•CH <sub>3</sub> •0.5H <sub>2</sub> O			
2 m m m 2 m m m 2	Ima2	C <sub>2v</sub> <sup>22</sup>	No. 46	Inorganic - 2 Organic - 3
Inorganic				
0.3975	H <sub>2</sub> Si <sub>2</sub> O <sub>5</sub>		0.7550	BaNa <sub>2</sub> Ti <sub>2</sub> Si <sub>4</sub> O <sub>14</sub>
Organic				
0.7831	AgC(CN) <sub>3</sub>		0.9811	(C <sub>9</sub> H <sub>6</sub> NS) <sub>2</sub> Zn
0.8722	Zn(NCS) <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub> ) <sub>2</sub>			
2 2 2 m m m	Pnmm	D <sub>2h</sub> <sup>1</sup>	No. 47	Inorganic - 11 Organic - 3
Inorganic				
0.4529	Ta <sub>4</sub> O		0.8639	Ca(UO <sub>2</sub> ) <sub>2</sub> (PO <sub>4</sub> ) <sub>2</sub> •0-2H <sub>2</sub> O
0.4614	BaSi <sub>3</sub> O <sub>3</sub>		0.8809	NbPt <sub>3</sub>
0.4629	RbBeF <sub>3</sub>		0.9420	Be <sub>2</sub> Ca(PO <sub>4</sub> ) <sub>2</sub>
0.6834	BiSeCl		0.9499	PbTi <sub>3</sub> O <sub>3</sub>
0.6941	CeCl <sub>3</sub> •7H <sub>2</sub> O		0.9635	Mg <sub>5</sub> (CO <sub>3</sub> ) <sub>4</sub> (OH) <sub>2</sub> •4H <sub>2</sub> O
0.8058	Ca(UO <sub>2</sub> ) <sub>2</sub> (PO <sub>4</sub> ) <sub>2</sub> •nH <sub>2</sub> O			
Organic				
0.6572	C <sub>14</sub> H <sub>10</sub> O <sub>4</sub>		0.9635	Mg <sub>5</sub> (CO <sub>3</sub> ) <sub>4</sub> (OH) <sub>2</sub> •4H <sub>2</sub> O
0.7010	C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>			
2 2 2 m m m	Pnnn	D <sub>2h</sub> <sup>2</sup>	No. 48	Inorganic - 1 Organic - 2
Inorganic				
0.6558	Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>2</sub> Si <sub>2</sub> O <sub>4</sub>			
Organic				
0.4000	C <sub>6</sub> H <sub>5</sub> NHNHC <sub>6</sub> H <sub>5</sub>		0.6854	[Cu(NC•CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CN) <sub>2</sub> ] <sub>2</sub> N <sub>2</sub>
2 2 2 m m m	Pccm	D <sub>2h</sub> <sup>3</sup>	No. 49	Inorganic - 0 Organic - 0
.....				

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	Pban	$D_{2h}^4$	No. 50	Inorganic - 3 Organic - 0
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## Inorganic

0.5630	$\text{Ca}[\text{B}(\text{OH})_4]_2$	0.9874	$\text{UO}_2(\text{OH})_2 \cdot \text{H}_2\text{O}$
0.8593	$\text{Sn}_4(\text{OH})_6\text{Cl}_2$		

## Organic

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$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	Pmma	$D_{2h}^5$	No. 51	Inorganic - 19 Organic - 2
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## Inorganic

0.1919	$\text{Ca}_2\text{Cu}_9(\text{OH})_{10}(\text{AsO}_4)_4 \cdot 10\text{H}_2\text{O}$	0.8661	$(\text{NH}_4)_2\text{HfF}_6$
0.2063	$[(\text{Cu}, \text{Pb})_5\text{Bi}_6\text{S}_{12}]$	0.8661	$(\text{NH}_4)_2\text{ZrF}_6$
0.5342	$\text{LiNb}_6\text{O}_{15}\text{F}$	0.9141	MoPt
0.5745	$\text{MgAlBO}_4$	0.9225	$7\text{UO}_3 \cdot 11\text{H}_2\text{O}$
0.6063	$\text{K}_2\text{Se}(\text{S}_2\text{O}_3)_2 \cdot 1.5\text{H}_2\text{O}$	0.9277	NbPt
0.7488	$\text{Rb}_2\text{S}_6$	0.9286	PtV
0.8065	$\text{CaCu}(\text{OH})\text{AsO}_4$	0.9414	$\text{KU}_3\text{F}_{13}$
0.8197	$\text{Re}_2\text{O}_7$	0.9497	CdMg
0.8653	$\text{Tl}_2\text{HfF}_6$	1.0000	$\text{Ni}_3\text{Al}_{10}\text{O}_{18}$
0.8657	$\text{Tl}_2\text{ZrF}_6$		

## Organic

0.5932	$(\text{C}_5\text{H}_{11})_4\text{NF} \cdot 3.6\text{H}_2\text{O}$	0.9098	$\text{NaHCN}_4 \cdot \text{H}_2\text{O}$
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$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	Pnna	$D_{2h}^6$	No. 52	Inorganic - 16 Organic - 5
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## Inorganic

0.3974	$\text{K}_2(\text{UO}_2)_2(\text{Si}_2\text{O}_5)_3 \cdot 4\text{H}_2\text{O}$	0.7816	$\text{Na}_2\text{S}_6$
0.5000	$\text{Mg}_6\text{Si}_{12}\text{O}_{32} \cdot 14\text{H}_2\text{O}$	0.8057	$\text{CaSnSi}_3\text{O}_{11}\text{H}_4$
0.5211	$\text{Ca}(\text{UO}_2)_2(\text{VO}_4)_2 \cdot 5-8.5\text{H}_2\text{O}$	0.8134	$\text{K}_2\text{Zr}_2\text{O}_5$
0.6120	$\text{LiSbO}_3$	0.8601	$\text{Mg}_2\text{Sn}$
0.7168	$\text{KMgCl}_3 \cdot 6\text{H}_2\text{O}$	0.9164	$\text{Ca}(\text{UO}_2)_2(\text{VO}_4)_2$
0.7285	$\text{Mn}_2\text{Mn}(\text{OH})_4(\text{AsO}_4)$	0.9304	$\text{K}_2\text{B}_{10}\text{H}_{10} \cdot x\text{H}_2\text{O}$
0.7334	$\text{K}_2\text{Pd}(\text{CN})_4 \cdot \text{H}_2\text{O}$	0.9774	$\text{GaCl}_2$
0.7801	$\text{Na}_2\text{CrO}_4$	0.9904	$\text{TlBr}_2$

## Organic

0.6292	$\text{Cu}(\text{C}_{10}\text{H}_8\text{N}_2)_2\text{Cl}_2 \cdot 6\text{H}_2\text{O}$	0.8822	$\text{C}_{20}\text{H}_{17}\text{N}_2\text{O}_3 \cdot 0.5(\text{HgCl}_4) \cdot \text{H}_2\text{O}$
0.7334	$\text{K}_2\text{Pd}(\text{CN})_4 \cdot \text{H}_2\text{O}$	0.9198	$\text{C}_{26}\text{H}_{18}\text{CuN}_2\text{O}_2$
0.8364	$\text{H}_2\text{UO}_4 \cdot (\text{NH}_2\text{CONH}_2)_2$		

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	Pmma	$D_{2h}^7$	No. 53	Inorganic - 16 Organic - 6
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## Inorganic

0.2966	$\text{Ca}_2(\text{Al}, \text{Fe})\text{Si}_3\text{AlO}_{10}(\text{OH})_2$	0.7510	CoEr <sub>3</sub>
0.3750	$\text{SbTlSe}_2$	0.7575	$\text{Se}(\text{SCN})_2$
0.3781	$(\text{As}, \text{Sb})_2\text{Tl}_2\text{Se}_4$	0.7947	$(\text{NH}_4)_2\text{S}_3\text{N}_2\text{O}_2$
0.3835	$\text{Tl}_2(\text{As}, \text{Sb})_2\text{Se}_4$	0.7987	$\text{Cu}_2\text{Fe}_2(\text{OH})_4(\text{AsO}_4)_2 \cdot \text{H}_2\text{O}$
0.4305	$\text{Ba}(\text{UO}_2)_3(\text{OH})_4(\text{SeO}_3)_2 \cdot 3\text{H}_2\text{O}$	0.9179	$\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$
0.5166	$\text{NaHgCl}_3$	0.9709	$\text{NH}_4\text{HF}_2$
0.6104	$\text{LiSbO}_3$	0.9772	$\text{NH}_4\text{HF}_2$
0.7159	GdSi	1.0000	$\text{Ca}_2\text{NaAl}_5\text{Si}_5\text{O}_{20} \cdot 6\text{H}_2\text{O}$

## Organic

0.4701	$\text{NH}_4\text{Cl} \cdot \text{NH}_2\text{CONH}_2$	0.6673	$\text{Cu}[\text{C}(\text{CN})_3]_2$
0.4856	$\text{CH}_2\text{OH}(\text{CH}_2\text{OH})_2\text{CH}_2\text{OH}$	0.7575	$\text{Se}(\text{SCN})_2$
0.6523	$(\text{Rh}(\text{CH}_3\text{COO})_2\text{Br})_2\text{Br}_2(\text{NH}_4)_4$	0.8669	$\text{Br}_2\text{C}_6\text{H}_2(\text{NH}_2)\text{COOH}$

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	Pcca	$D_{2h}^8$	No. 54	Inorganic - 5 Organic - 0
Inorganic				
0.5853	$Li_2Ge_4O_9$		0.7947	$RbMnCl_3 \cdot 2H_2O$
0.7760	$AgBa(NO_2)_3 \cdot H_2O$		0.9177	$AgClO_2$
0.7909	$CsMnCl_3 \cdot 2H_2O$			
Organic				
.....				

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	Pbam	$D_{2h}^9$	No. 55	Inorganic - 36 Organic - 3
Inorganic				
0.3779	$PdSn_3$		0.7607	$Fe_4B_2V_2O_{10}$
0.5045	$Al_3Pt_5$		0.7610	$Fe_2FeBO_5$
0.5048	$Au_2CuZn$		0.7618	$Co_4Fe_2B_2O_{10}$
0.5133	$Ga_3Pd_5$		0.7641	$Co_2Co(BO_3)_2O_2$
0.5136	$B_2C_2Sc$		0.7644	$K_2HgCl_4 \cdot H_2O$
0.5248	$Rh_5Si_3$		0.7661	$B_2Fe_4(Fe, Mg)_2O_{13}$
0.5252	$Ge_3Rh_5$		0.7693	$Fe_2FeBO_5$
0.5253	$Li_7Si_2$		0.7704	$Fe_6B_2O_{10}$
0.6883	$As_2Ge$		0.7821	$Cu_4Fe_2B_2O_{10}$
0.6946	$NbBr_5$		0.7874	$(Fe, Mg)_2FeBO_5$
0.6997	$NbBr_5$		0.8578	$Dy_2Mn_4O_9$
0.7122	$TaBr_5$		0.8664	$HoMn_2O_5$
0.7341	$Mg_3(Mg_{1-x}Fe_x)Fe_2B_2O_{10}$		0.8768	$BiMn_2O_5$
0.7546	$Fe_2Ni_4B_2O_{10}$		0.8850	$NH_2S_3H$
0.7553	$FeMg_2BO_5$		0.9521	$Bi_2Al_4O_9$
0.7587	$(Fe, Mg)_2FeBO_5$		0.9770	$B_8Ru_{11}$
0.7596	$FeMg_2BO_5$		0.9812	$Al_6Si_2O_{13}$
0.7597	$Co_4B_2V_2O_{10}$		0.9872	$Al_4Si_6O_8$
Organic				
0.5136	$B_2ScC_2$		0.9410	$K_2Ni(O_2NN(CH_2)_3NNO_2)_2 \cdot 4H_2O$
0.6029	$(C_2H_4PdCl_2)_2$			

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	Pccn	$D_{2h}^{10}$	No. 56	Inorganic - 11 Organic - 29
Inorganic				
0.3647	$Pb(I_3)_2$		0.8844	$(Nb_6I_8)I_3$
0.4350	$Sb_2O_3$		0.8870	$(Nb_6I_8)I_3$
0.8119	$(NH_4)HCO_3$		0.8957	$B_{18}H_{22}$
0.8155	$(NH_4)_2H_2P_2O_6$		0.9139	$B_{10}H_{12}I_2$
0.8178	$(NH_4)_2H_2P_2O_6$		0.9805	$(NH_4)_6TeMo_6O_{24} \cdot 7H_2O$
0.8234	$BaHPO_4$			
Organic				
0.2589	$C_{15}H_{28}$		0.7000	$(CH_3C_6H_4Si_1.5)_8$
0.2598	$(BrC_6H_4CF)_2$		0.7039	$ClC_6H_3(N_2)_2$
0.4091	$C_6H_5NH_3Br$		0.7094	$AgP_2(O_2C_2H_5)_2$
0.4204	$Zn(NO_3)_2 \cdot 4[(NH_2)_2CS]$		0.7137	$BrC_6H_3(N_2)_2$
0.4826	$ClHgCO_3 \cdot CH_3$		0.8105	$[(H_2N)_2CS]_2I_2 \cdot H_2O$
0.5005	$CH_3 \cdot CO \cdot NH_2$		0.8119	$(NH_4)HCO_3$
0.5086	$UO_2(C_5H_7O_2)_2 \cdot H_2O$		0.8484	$[(C_2H_5)_2PSSe]_2$
0.5227	$(Cl \cdot C_6H_4)_2P(O)(OH)$		0.8528	$U[(C_6H_5CO)_2CH]_4$
0.5427	$[(CH_3)_3AsPdClBr]_2$		0.8552	$Ce[(C_6H_5CO)_2CH]_4$
0.5927	$Cu(HCOCH_2CH_2NH_2)_2 \cdot S_2O_4 \cdot 4H_2O$		0.8661	$C_6(C_6OH)_6$
0.6159	$C_{10}H_4Cl_4$		0.8699	$Th[(C_6H_5CO)_2CH]_4$
0.6639	$CH_2=CH-CO-NH-CO-\theta-CH_3$		0.9169	$C_{12}H_{26}N_2 \cdot 2HBr$
0.6670	$S(CH_2CH_2CN)_2$		0.9426	$Fe(CO)_4 \cdot C_4H_4O_4$
0.6803	$Co_4(CO)_{12}$		0.9570	$(CH_3)_2CBNH_2 \cdot Au \cdot C \cdot C \cdot C_6H_5$
0.6845	$Te(C_4H_8N_2S)_2(S_2O_2CH_3)_2$			

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	Pbcm	$D_{2h}^{11}$	No. 57	Inorganic - 22 Organic - 21
Inorganic				
0.4720	RbV $\theta_3$		0.7514	Ba <sub>2</sub> Tl(N $\theta_2$ ) <sub>5</sub>
0.4744	CeV $\theta_3$		0.8664	[(NH <sub>4</sub> ) <sub>3</sub> ClS <sub>2</sub> $\theta_6$ ]
0.4763	NH <sub>4</sub> V $\theta_3$		0.8786	KCNS
0.4906	PBr <sub>5</sub>		0.9041	TlCNS
0.5088	AlDy		0.9319	Pb $\theta$
0.5172	Hg <sub>7</sub> K <sub>5</sub>		0.9665	Mo $\theta_2$ (P $\theta_3$ ) <sub>2</sub>
0.5268	KV $\theta_3$		0.9681	CaMn <sub>2</sub> $\theta_4$
0.6247	Hg <sub>2</sub> ( $\theta$ H) <sub>2</sub> (Br $\theta_3$ ) <sub>2</sub>		0.9802	NH <sub>2</sub> NBS $\theta_3$ H
0.6255	Hg <sub>2</sub> ( $\theta$ H) <sub>2</sub> (Cl $\theta_3$ ) <sub>2</sub>		0.9877	BaU $\theta_4$
0.6460	Ca <sub>2</sub> Cl(P $\theta_4$ )		0.9886	AuTlTe
0.7110	CaCr $\theta_4$ •2H <sub>2</sub> $\theta$		0.9963	KNH <sub>2</sub> S $\theta_3$
Organic				
0.0962	C <sub>25</sub> H <sub>60</sub>		0.7283	C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> C $\theta\theta$ H
0.1030	C <sub>27</sub> H <sub>56</sub>		0.8582	CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N:NC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub>
0.1109	C <sub>25</sub> H <sub>52</sub>		0.8776	Mo $\theta_3$ (NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> NH
0.1200	C <sub>23</sub> H <sub>48</sub>		0.8786	KCNS
0.1305	C <sub>21</sub> H <sub>44</sub>		0.9041	TlCNS
0.3028	C <sub>6</sub> H <sub>5</sub> C $\theta$ NHC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub>		0.9364	C <sub>10</sub> H <sub>4</sub> (N $\theta_2$ ) <sub>4</sub>
0.4878	C <sub>4</sub> H <sub>3</sub> $\theta_4$ K		0.9504	HgCl <sub>2</sub> •C <sub>3</sub> H <sub>6</sub> S <sub>3</sub>
0.6599	C(CN) <sub>3</sub> Br		0.9527	C <sub>6</sub> H <sub>3</sub> $\theta$ H(N $\theta_2$ ) <sub>2</sub>
0.6698	AgN $\theta_3$ •C <sub>3</sub> H <sub>6</sub> S <sub>3</sub> •H <sub>2</sub> $\theta$		0.9928	C <sub>26</sub> H <sub>16</sub> S <sub>2</sub>
0.6865	Cu <sub>4</sub> (NH <sub>2</sub> CSNH <sub>2</sub> ) <sub>9</sub> (N $\theta_3$ ) <sub>4</sub>		0.9980	C <sub>5</sub> H <sub>11</sub> N•HCl
0.6955	N $\theta_2$ C <sub>6</sub> H <sub>4</sub> NHC <sub>6</sub> H <sub>5</sub>			

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	Pnmm	$D_{2h}^{12}$	No. 58	Inorganic - 59 Organic - 10
Inorganic				
0.3464	PdCl <sub>2</sub>		0.8418	CoTe <sub>2</sub>
0.4176	InS		0.8435	FeTe <sub>2</sub>
0.4968	BaGeSe <sub>3</sub>		0.8462	CoSe <sub>2</sub>
0.5222	(Mg,Li) <sub>7</sub> Si $\theta_2$ 2F <sub>2</sub>		0.8497	Mn $\theta$ ( $\theta$ H)
0.5926	Ca <sub>1.6</sub> (Mg,Mn,Ba) <sub>0.5</sub> Si $\theta_4$		0.8520	Zr <sub>4</sub> ( $\theta$ H) <sub>6</sub> (Cr $\theta_4$ ) <sub>5</sub> •2H <sub>2</sub> $\theta$
0.5973	Ca <sub>2</sub> Si $\theta_4$		0.8530	FeTe <sub>2</sub>
0.6247	S <sub>12</sub>		0.8669	In $\theta$ ( $\theta$ H)
0.6414	Mg <sub>3</sub> (B $\theta_3$ ) <sub>2</sub>		0.8754	CrSb <sub>2</sub>
0.6430	Ni <sub>3</sub> (B $\theta_3$ ) <sub>2</sub>		0.8792	FeP <sub>2</sub>
0.6470	Mn <sub>3</sub> (B $\theta_3$ ) <sub>2</sub>		0.8829	Cr $\theta\theta$ H
0.6475	Co <sub>3</sub> (B $\theta_3$ ) <sub>2</sub>		0.8857	As <sub>5</sub> Mo
0.6523	BiCl <sub>1.167</sub>		0.8858	As <sub>2</sub> Fe
0.6752	As <sub>2</sub> Ti		0.8886	AsSb <sub>2</sub>
0.6920	E <sub>10</sub> H <sub>14</sub>		0.8935	RuSb <sub>2</sub>
0.7661	Na <sub>2</sub> [N $\theta$ (CN) <sub>5</sub> Co] <sub>2</sub> •2H <sub>2</sub> $\theta$		0.9006	CrCl <sub>2</sub>
0.7673	Na <sub>2</sub> Fe(CN) <sub>5</sub> (N $\theta$ )•2H <sub>2</sub> $\theta$		0.9321	Ge <sub>2</sub> Pt
0.7690	Na $\theta_2$		0.9433	Co <sub>2</sub> N
0.7879	B <sub>6</sub> Si		0.9582	CaBr <sub>2</sub>
0.8008	P <sub>4</sub> Ta <sub>5</sub>		0.9585	Cu <sub>2</sub> ( $\theta$ H)P $\theta_4$
0.8008	BaU $\theta_6$ <sub>19</sub> •10-11H <sub>2</sub> $\theta$		0.9619	Na <sub>14</sub> Nb <sub>12</sub> $\theta_37$ •32H <sub>2</sub> $\theta$
0.8012	PTa <sub>2</sub>		0.9705	CaCl <sub>2</sub>
0.8095	CuSe <sub>2</sub>		0.9742	Zn(Zn $\theta$ H)As $\theta_4$
0.8110	CuSe <sub>2</sub>		0.9764	Zn(Zn $\theta$ H)As $\theta_4$
0.8159	K <sub>2</sub> U $\theta_6$ <sub>19</sub> •11H <sub>2</sub> $\theta$		0.9800	SnCl <sub>4</sub> •2P $\theta$ Cl <sub>3</sub>
0.8193	FeS <sub>2</sub>		0.9823	Al <sub>2</sub> Si $\theta_5$
0.8205	NiSe <sub>2</sub>		0.9830	CCo <sub>2</sub>
0.8212	As <sub>2</sub> Ni		0.9868	Al <sub>2</sub> Si $\theta_5$
0.8216	(Co,Ni,Fe)AsS		0.9926	TiCl <sub>4</sub> •2P $\theta$ Cl <sub>3</sub>
0.8270	As <sub>2</sub> Ni		0.9987	Al <sub>2</sub> $\theta$ Si $\theta_4$
0.8399	FeSe <sub>2</sub>			
Organic				
0.4768	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> PbCl <sub>2</sub>		0.7661	Na <sub>2</sub> [N $\theta$ (CN) <sub>5</sub> Co] <sub>2</sub> •2H <sub>2</sub> $\theta$
0.4817	CdBr <sub>2</sub> •2(C <sub>5</sub> H <sub>5</sub> N)		0.7673	Na <sub>2</sub> Fe(CN) <sub>5</sub> (N $\theta$ )•2H <sub>2</sub> $\theta$
0.6345	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>		0.8004	[(NH <sub>3</sub> ) <sub>5</sub> Co $\theta_2$ Co(NH <sub>3</sub> ) <sub>5</sub> ](NCS) <sub>4</sub>
0.6632	C <sub>6</sub> H <sub>5</sub> C $\theta$ CC $\theta\theta$ H		0.9192	Au(C <sub>4</sub> H <sub>7</sub> N <sub>2</sub> $\theta_2$ ) <sub>2</sub> •AuCl <sub>2</sub>
0.7476	CuCl <sub>2</sub> •(NH <sub>2</sub> C $\theta$ NHC $\theta$ NH <sub>2</sub> ) <sub>2</sub>		0.9830	Co <sub>2</sub> C

$\begin{matrix} 2 & 2 & 2 \\ m & m & m \end{matrix}$	Pmmn	$D_{2h}^{13}$	No. 59	Inorganic - 38 Organic - 15
Inorganic				
0.2325	AsMn <sub>3</sub>		0.6637	Pb <sub>6</sub> FeBi <sub>4</sub> Sb <sub>2</sub> S <sub>16</sub>
0.3559	Cu <sub>2</sub> Pb <sub>5</sub> (OH) <sub>6</sub> Ce <sub>3</sub> (SO <sub>4</sub> ) <sub>3</sub>		0.7098	KSbF <sub>4</sub>
0.3796	V <sub>2</sub> O <sub>5</sub>		0.8036	Au <sub>3</sub> Zr
0.4300	KTi <sub>3</sub> NbO <sub>9</sub>		0.8282	(Hg <sub>2</sub> N <sub>2</sub> H <sub>2</sub> )Cl <sub>2</sub>
0.4329	BaTi <sub>4</sub> O <sub>9</sub>		0.8655	Cu <sub>3</sub> Sb
0.4362	ZrNi		0.8673	Hg(OH)F
0.4619	CrOBr		0.8676	AlCu <sub>3</sub>
0.4681	InOBr		0.8704	B <sub>2</sub> Os
0.4698	Al <sub>3</sub> Mn(AlOH) <sub>2</sub> Mn <sub>4</sub> (SiO <sub>4</sub> ) <sub>5</sub> (As, V) <sub>4</sub> •2H <sub>2</sub> O		0.8709	B <sub>2</sub> Ru
0.4717	FeOCl		0.8753	Ba <sub>2</sub> [Fe, Ti, Fe, Mg] <sub>2</sub> [O(Si <sub>4</sub> O <sub>12</sub> )]•H <sub>2</sub> O
0.4720	AlOCl		0.8763	Cu <sub>3</sub> Ti
0.4754	Mn <sub>8</sub> Al <sub>8</sub> V <sub>2</sub> Si <sub>3</sub> O <sub>35</sub> •5H <sub>2</sub> O		0.8784	MoNi <sub>3</sub>
0.5031	InOCl		0.8865	(Nb <sub>0.75</sub> Ti <sub>0.25</sub> )Ni <sub>3</sub>
0.5103	Mn <sub>5</sub> (OH) <sub>4</sub> (AsO <sub>4</sub> ) <sub>2</sub>		0.8871	(Ni <sub>0.67</sub> Cu <sub>0.33</sub> ) <sub>3</sub> Ti
0.5263	UO <sub>2</sub> Ce <sub>3</sub>		0.9284	AsCuPbS <sub>3</sub>
0.5789	AgFe <sub>2</sub> S <sub>3</sub>		0.9478	NH <sub>4</sub> N <sub>3</sub>
0.5885	CuTe		0.9514	Cu <sub>2</sub> (OH)AsO <sub>4</sub>
0.5887	CuTe		0.9635	BrCN
0.6228	Y <sub>3</sub> O(OH) <sub>5</sub> Cl <sub>2</sub>		0.9902	CCLN
Organic				
0.3865	Na <sub>2</sub> [SO <sub>3</sub> CH(OH)•CH <sub>2</sub> •CH <sub>2</sub> SO <sub>3</sub> ]•4H <sub>2</sub> O		0.8849	[(CH <sub>3</sub> ) <sub>4</sub> Sb][Fe(O•Si[CH <sub>3</sub> ] <sub>3</sub> ) <sub>4</sub> ]
0.4716	Ce(NHCH <sub>3</sub> ) <sub>2</sub>		0.8858	[(CH <sub>3</sub> ) <sub>4</sub> Sb][Al(O•Si[CH <sub>3</sub> ] <sub>3</sub> ) <sub>4</sub> ]
0.5035	HgCl <sub>2</sub> (N <sub>2</sub> H <sub>4</sub> CS) <sub>2</sub>		0.8874	[(CH <sub>3</sub> ) <sub>4</sub> Sb][Ga(O•Si[CH <sub>3</sub> ] <sub>3</sub> ) <sub>4</sub> ]
0.5263	UO <sub>2</sub> Ce <sub>3</sub>		0.9027	CH <sub>3</sub> C•NHCH <sub>3</sub>
0.6840	C <sub>4</sub> H <sub>7</sub> O <sub>4</sub> N		0.9635	BrCN
0.8008	C <sub>14</sub> H <sub>8</sub> O <sub>2</sub>		0.9773	(C <sub>6</sub> H <sub>4</sub> C•OH) <sub>2</sub>
0.8028	C <sub>6</sub> H <sub>5</sub> Br		0.9902	CNCl
0.8251	C <sub>6</sub> H <sub>5</sub> Cl			

$\begin{matrix} 2 & 2 & 2 \\ m & m & m \end{matrix}$	Pbcn	$D_{2h}^{14}$	No. 60	Inorganic - 119 Organic - 65
Inorganic				
0.3617	BaS <sub>2</sub> O <sub>3</sub> •H <sub>2</sub> O		0.3995	MgNb <sub>2</sub> O <sub>6</sub>
0.3672	BaS <sub>2</sub> O <sub>3</sub> •H <sub>2</sub> O		0.4003	Mn(Ta, Nb) <sub>2</sub> O <sub>6</sub>
0.3731	LaTi <sub>1.5</sub> Mo <sub>0.5</sub> O <sub>6</sub>		0.4007	MnNb <sub>2</sub> O <sub>6</sub>
0.3788	CeNbTiO <sub>6</sub>		0.4017	K[AsF <sub>6</sub> (OH)]
0.3790	Lu(Nb, Ti) <sub>2</sub> O <sub>6</sub>		0.4023	FeNb <sub>2</sub> O <sub>6</sub>
0.3792	LuNbTiO <sub>6</sub>		0.4024	(Fe, Mn)(Nb, Ta) <sub>2</sub> O <sub>6</sub>
0.3794	Tm(Nb, Ti) <sub>2</sub> O <sub>6</sub>		0.4030	ZnNb <sub>2</sub> O <sub>6</sub>
0.3795	Yb(Nb, Ti) <sub>2</sub> O <sub>6</sub>		0.4036	ZnTa <sub>2</sub> O <sub>6</sub>
0.3798	Er(Nb, Ti) <sub>2</sub> O <sub>6</sub>		0.4038	CoNb <sub>2</sub> O <sub>6</sub>
0.3799	YbNbTiO <sub>6</sub>		0.4041	NiNb <sub>2</sub> O <sub>6</sub>
0.3800	ErNbTiO <sub>6</sub>		0.4045	MnSb <sub>2</sub> O <sub>6</sub>
0.3801	TmNbTiO <sub>6</sub>		0.4051	Fe <sub>2</sub> WO <sub>6</sub>
0.3801	Y(Nb, Ti) <sub>2</sub> O <sub>6</sub>		0.4077	LiWV <sub>2</sub> O <sub>7.5</sub>
0.3802	Yb(Ta, Ti) <sub>2</sub> O <sub>6</sub>		0.4287	UCrO <sub>4</sub>
0.3802	Dy(Nb, Ti) <sub>2</sub> O <sub>6</sub>		0.4436	BivO <sub>4</sub>
0.3803	Ho(Nb, Ti) <sub>2</sub> O <sub>6</sub>		0.4507	Tl <sub>2</sub> S <sub>5</sub>
0.3807	Tb(Nb, Ti) <sub>2</sub> O <sub>6</sub>		0.4626	K <sub>2</sub> Pb(NO <sub>2</sub> ) <sub>4</sub> •H <sub>2</sub> O
0.3808	YTiTaO <sub>6</sub>		0.4897	CaHAsO <sub>4</sub> •H <sub>2</sub> O
0.3808	Er(Ta, Ti) <sub>2</sub> O <sub>6</sub>		0.4913	CaHAsO <sub>4</sub> •H <sub>2</sub> O
0.3808	GdNbTiO <sub>6</sub>		0.4916	CaHAsO <sub>4</sub> •H <sub>2</sub> O
0.3809	DyNbTiO <sub>6</sub>		0.5336	CaB <sub>2</sub> O <sub>4</sub>
0.3810	YNbTiO <sub>6</sub>		0.5355	CaB <sub>2</sub> O <sub>4</sub>
0.3810	TbNbTiO <sub>6</sub>		0.5472	SrB <sub>2</sub> O <sub>4</sub>
0.3812	Y(Ta, Ti) <sub>2</sub> O <sub>6</sub>		0.5827	Li <sub>2</sub> Ge <sub>7</sub> O <sub>15</sub>
0.3812	GdNbTiO <sub>6</sub>		0.5892	Rb <sub>2</sub> Te(S <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> •1.5H <sub>2</sub> O
0.3814	(Er, Nd)(Nb, Ti) <sub>2</sub> O <sub>6</sub>		0.5936	Cs <sub>2</sub> Te(S <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> •1.5H <sub>2</sub> O
0.3817	YNbTiO <sub>6</sub>		0.5938	Cu[Hg(CNS) <sub>4</sub> ]
0.3817	Gd(Nb, Ti) <sub>2</sub> O <sub>6</sub>		0.5951	Th(P <sub>2</sub> O <sub>3</sub> ) <sub>4</sub>
0.3835	CaNb <sub>2</sub> O <sub>6</sub>		0.5986	Rb <sub>2</sub> Se(S <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> •1.5H <sub>2</sub> O
0.3835	(Ca, TR)(Nb, Ti) <sub>2</sub> (O, OH) <sub>6</sub>		0.5991	U(P <sub>2</sub> O <sub>3</sub> ) <sub>4</sub>
0.3941	CdTa <sub>2</sub> O <sub>6</sub>		0.5997	Pu(P <sub>2</sub> O <sub>3</sub> ) <sub>4</sub>
0.3953	Cd(NbO <sub>3</sub> ) <sub>2</sub>		0.6009	Rb <sub>2</sub> S(S <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> •1.5H <sub>2</sub> O
0.3987	(Mg, Fe, Mn)(Nb, Ta) <sub>2</sub> O <sub>6</sub>		0.6010	Na <sub>2</sub> Ti <sub>2</sub> Si <sub>2</sub> O <sub>9</sub>
0.3990	MnTa <sub>2</sub> O <sub>6</sub>		0.6037	Na <sub>2</sub> (Ti, Zr) <sub>2</sub> Si <sub>2</sub> O <sub>9</sub>
0.3993	MnTa <sub>2</sub> O <sub>6</sub>		0.6110	(NH <sub>4</sub> ) <sub>2</sub> Se(S <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> •1.5H <sub>2</sub> O
0.3994	Mn(Ta, Nb, Ti) <sub>2</sub> O <sub>6</sub>		0.6120	K <sub>2</sub> S(S <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> •1.5H <sub>2</sub> O

Pbcn  $D_{2h}^{14}$  No. 60 (continued)

## Inorganic (continued)

0.6124	$(NH_4)_2S_5O_6 \cdot 1.5H_2O$	0.8351	$(Mn, Fe)(Ta, Nb, Ti, Sn)_2O_6$
0.6438	$KPtNH_3Cl_3 \cdot H_2O$	0.8381	$Ca_4[U(NCS)_8] \cdot 2H_2O$
0.6631	$K(PtNH_3Br_3) \cdot H_2O$	0.8524	$ReO_2$
0.6699	$KPtNH_3Br_3 \cdot H_2O$	0.8659	$CrO_2$
0.6819	$Cr_5O_{12}$	0.8772	$Cu_2$
0.6992	$In_2(WO_4)_3$	0.8788	$UO_3 \cdot 2H_2O$
0.7068	$PrSc(WO_4)_3$	0.8788	$Na_4XeO_6 \cdot 8H_2O$
0.7143	$In_2(MoO_4)_3$	0.8810	$UO_3 \cdot (2-x)H_2O$
0.7176	$ScYb(WO_4)_3$	0.8859	$NiNb_2O_6$
0.7187	$Fe_2(MoO_4)_3$	0.8912	$TiO_2$
0.7199	$Sc_2(WO_4)_3$	0.8913	$GaTaO_4$
0.7200	$Al_2(MoO_4)_3$	0.8990	$(Ta, Fe, Sn, Nb, Mn)O_2$
0.7222	$Cr_2(MoO_4)_3$	0.9130	$ZnF_2$
0.7241	$Yb_2(WO_4)_3$	0.9153	$PbO_n$
0.7254	$Rh_2S_3$	0.9237	$PbO_2$
0.7272	$Sc_2(MoO_4)_3$	0.9272	$Mn(II)_{1-x}[Fe(III)(OH)_x]_3[(3-3x)(H_2O)](PO_4)_2$
0.7278	$Sc_2(MoO_4)_3$	0.9359	$CoNb_2O_6$
0.7280	$Al_2(WO_4)_3$	0.9391	$(Fe, Mn)_3(PO_4)_2 \cdot 3H_2O$
0.7686	$K_3Ir(CN)_6$	0.9419	$(Mn, Fe)_3(PO_4)_2 \cdot 3H_2O$
0.7755	$K_3[Fe(CN)_6]$	0.9449	$MgSiO_3$
0.7761	$K_3[Co(CN)_6]$	0.9515	$Cu_8(Si_4O_{11})_2(OH)_4 \cdot H_2O$
0.7815	$K_3Mn(CN)_6$	0.9965	$F_4S_{6.5}$
0.7823	$K_3Cr(CN)_6$	1.0000	$(N_2H_5)_2SnCl_6$
0.8176	$Na_7MnH_4(I_6)_3 \cdot 17H_2O$		

## Organic

0.1220	$CH_3(CH_2)_5CO \cdot C_6H_5Na$	0.7761	$K_3[Co(CN)_6]$
0.1376	$CH_3(CH_2)_4CO \cdot C_6H_5Na$	0.7815	$K_3Mn(CN)_6$
0.1801	$CH_3(CH_2)_2CO \cdot C_6H_5Na$	0.7823	$K_3Cr(CN)_6$
0.2065	$CH_3CH_2CO \cdot C_6H_5Na$	0.7977	$B_{10}Cl_8H_2C_2H_2$
0.2880	$(BrC_6H_4)_2O \cdot (CH_3C_6H_4)_2CO$	0.8010	$C_{18}H_{10}(CH_3)_2$
0.3620	$KS_3 \cdot CHCl \cdot CO \cdot K \cdot 1.5H_2O$	0.8079	$(CH_3CO)_4C_2H_2$
0.3899	$K_2(C_6H_5)_2PF_6 \cdot 1.5H_2O$	0.8104	$C_{12}H_{10}N_2$
0.3966	$C_{12}H_4N_2O_2Br_6$	0.8169	$CaY(F_3COCH_2CF_3)_4$
0.4567	$C_2H_5Li$	0.8289	$C_6H_5OH \cdot 0.5H_2O$
0.4660	$C_4H_2O_4$	0.8381	$Ca_4[U(NCS)_8] \cdot 2H_2O$
0.4667	$(C_6H_4 \cdot CO \cdot C_6H_4)_2$	0.8407	$C_{15}H_5N_5O_6$
0.4739	$C_{13}H_8Br_2O$	0.8519	$C_6H_5 \cdot CO \cdot CH \cdot C_6H_5$
0.4830	$BrC_6H_4 \cdot CO \cdot CH_2 \cdot CO \cdot C_6H_4Br$	0.8520	$Mn(C_{13}H_{15}N_2O_4) \cdot 4H_2O$
0.5147	$(C_{12}H_{18})_2AgNO_3$	0.8536	$P_2C_2H_2N_2Mo(CO)_4$
0.5167	$C_8H_8Cl_2N_2O_2$	0.8623	$Zr(C_6H_5N_2O_2)_4$
0.5310	$CO(NH_2)_2 \cdot 2H_2O$	0.8659	$Mo_2C$
0.5412	$(C_6H_5)_2SbCl_3$	0.8772	$V_2C$
0.5457	$C_{10}H_{12}O_2$	0.8877	$C_2H_4Se_2O_3$
0.5778	$Be_4O(C_6H_5COO)_6$	0.8984	$C_6H_5 \cdot CH \cdot N \cdot ON \cdot CH \cdot C_6H_5$
0.5798	$C_{16}H_{32}N_4 \cdot Ni(ClO_4)_2$	0.8984	$[CH_3SC(NH_2)_2]_2SO_4$
0.5938	$Cu[Hg(CNS)_4]$	0.8988	$C_{12}H_{10} \cdot C_6(N_2O_2)_3$
0.5943	$C_{16}H_{28}N_4 \cdot Ni(ClO_4)_2$	0.9058	$(C_6H_5)_2SeBr_2$
0.6151	$C_5H_{12}$	0.9164	$Te((CH_3O)_2PS_2)_2$
0.6598	$C_{13}H_9 \cdot NO \cdot xH_2O$	0.9200	$C_6H_5NO$
0.6842	$(Cl \cdot C_6H_3 \cdot NH_2)_2$	0.9212	$Pt(C_6H_4[As(CH_3)_2]_2)_2Cl_2$
0.6910	$HO \cdot C \cdot CH \cdot CO \cdot C_6H_5$	0.9212	$Pt[(CH_3)_2AsH]_2Cl_2$
0.7140	$(CH_3SO_2)_2C_2C \cdot NO \cdot CH_3$	0.9293	$Cu(C_5H_5N)_2SO_4 \cdot 2H_2O$
0.7369	$(C_{14}H_8NO)_2$	0.9714	$C_{10}H_{12}S_4O_2$
0.7525	$[(C_5H_5)_2TiAl(C_2H_5)_2]_2$	0.9814	$[(CH_3)_3SO]BF_4$
0.7686	$K_3Ir(CN)_6$	0.9978	$Pt(NH_3)_2(SCN)_2$
0.7700	$C_{20}H_{16}O_6$	0.9992	$C_8H_8Cl_6N_6$
0.7732	$Te(C_6H_5S_2O_2)_2$	1.0000	$[SC(CH_3)_3]_2Si[Sch(CH_3)_2]_2$
0.7755	$K_3[Fe(CN)_6]$		

 $\frac{2}{m} \frac{2}{m} \frac{2}{m}$ Pbca  $D_{2h}^{15}$  No. 61Inorganic - 98  
Organic - 210

## Inorganic

0.2414	$MgSiO_3$	0.4790	$CoGeO_3$
0.3057	$(Tl, Pb)_2As_5S_9$	0.4803	$MnGeO_3$
0.3924	$KH_5O_8$	0.4835	$[MgSiO_3]$
0.4736	$NaAsO_2$	0.4852	$MgSiO_3$
0.4754	$BeO_2 \cdot 2H_2O$	0.4854	$Mg(NH_4)_2H_2(PO_4)_2 \cdot 4H_2O$
0.4757	$TeO_2$	0.4868	$(Mg, Fe)SiO_3$
0.4785	$AgIO_3$	0.4875	$FeMgSi_2O_6$

Pbca  $D_{2h}^{15}$  No. 61 (continued)

## Inorganic (continued)

0.4875	Cd(N <sub>3</sub> ) <sub>2</sub>	0.7834	Cu <sub>2</sub> B <sub>10</sub> H <sub>10</sub>
0.4885	MgSi <sub>3</sub>	0.7886	(NH <sub>4</sub> ) <sub>10</sub> W <sub>12</sub> O <sub>41</sub> •11H <sub>2</sub> O
0.4926	FeSi <sub>3</sub>	0.7936	KB <sub>5</sub> O <sub>8</sub>
0.4985	Cu <sub>5</sub> (Si <sub>3</sub> O <sub>7</sub> ) <sub>4</sub> (OH) <sub>2</sub>	0.7995	Be <sub>2</sub> (OH)B <sub>6</sub> O <sub>3</sub>
0.5065	LaSI	0.8000	RbB <sub>5</sub> O <sub>8</sub>
0.5108	CeSI	0.8286	TcCl <sub>4</sub>
0.5113	As <sub>2</sub> Ni	0.8600	BiOHCrO <sub>4</sub>
0.5139	LaSBr	0.8744	U <sub>6</sub> O <sub>3</sub> •2H <sub>2</sub> O
0.5142	LaSCL	0.8768	HSO <sub>3</sub> NH <sub>2</sub>
0.5150	MgP <sub>6</sub> O <sub>10</sub> •5H <sub>2</sub> O	0.8773	U <sub>6</sub> O <sub>3</sub> •(2+?)H <sub>2</sub> O
0.5151	CeSBr	0.8781	NiP
0.5166	Mg <sub>2</sub> B <sub>10</sub> O <sub>17</sub> •8H <sub>2</sub> O	0.8800	NNO <sub>3</sub> •2BF <sub>3</sub>
0.5172	KHSO <sub>4</sub>	0.8829	H <sub>3</sub> N•BF <sub>3</sub>
0.5200	CeSCL	0.8868	2NO <sub>2</sub> •3SO <sub>3</sub>
0.5261	KAg(NCSe) <sub>2</sub>	0.8972	CaCO <sub>3</sub>
0.5299	NaOH•H <sub>2</sub> O	0.8984	CaPd(CN) <sub>4</sub> •5H <sub>2</sub> O
0.5479	Na <sub>4</sub> XeO <sub>6</sub> •6H <sub>2</sub> O	0.8995	CaPt(CN) <sub>4</sub> •5H <sub>2</sub> O
0.5808	Zn(OH)Cl	0.9043	U <sub>6</sub> O <sub>3</sub> •(2-?)H <sub>2</sub> O
0.5879	FeOHCl	0.9090	Na <sub>6</sub> Si <sub>2</sub> O <sub>7</sub> •11H <sub>2</sub> O
0.5906	SrHAsO <sub>4</sub> •H <sub>2</sub> O	0.9132	S <sub>6</sub> (NH) <sub>2</sub>
0.5913	TiO <sub>2</sub>	0.9293	[(NH <sub>3</sub> ) <sub>5</sub> Co-O <sub>2</sub> -Co(NH <sub>3</sub> ) <sub>5</sub> ](NO <sub>3</sub> ) <sub>4</sub> •HF <sub>2</sub> •(H <sub>2</sub> O) <sub>2</sub>
0.5942	TiO <sub>2</sub>	0.9323	LiB(OH) <sub>4</sub>
0.5969	AuSn <sub>2</sub>	0.9539	SbZn
0.5980	(NH <sub>4</sub> ) <sub>2</sub> Cr <sub>3</sub> O <sub>10</sub>	0.9554	MgHP <sub>4</sub> O <sub>4</sub> •3H <sub>2</sub> O
0.6135	CdB <sub>4</sub> O <sub>7</sub>	0.9558	SbZn
0.6278	MgB <sub>4</sub> O <sub>7</sub>	0.9564	MgHP <sub>4</sub> O <sub>4</sub> •3H <sub>2</sub> O
0.6285	U <sub>6</sub> O <sub>3</sub> (OH) <sub>2</sub>	0.9565	K <sub>6</sub> TeMo <sub>6</sub> O <sub>24</sub> •7H <sub>2</sub> O
0.6336	U <sub>6</sub> O <sub>3</sub> (OH) <sub>2</sub>	0.9607	Rb <sub>2</sub> Se(SO <sub>3</sub> ) <sub>2</sub>
0.6351	CaCrO <sub>4</sub> •H <sub>2</sub> O	0.9680	CdSb
0.6462	B <sub>2</sub> Cl <sub>4</sub>	0.9695	AlH <sub>2</sub> (OH) <sub>2</sub> P <sub>4</sub>
0.6718	S(CN) <sub>2</sub>	0.9718	FeAsO <sub>4</sub> •2H <sub>2</sub> O
0.6898	Na <sub>2</sub> (NH <sub>4</sub> ) <sub>8</sub> W <sub>12</sub> O <sub>41</sub> •13H <sub>2</sub> O	0.9727	FeAsO <sub>4</sub> •2H <sub>2</sub> O
0.6899	(NH <sub>4</sub> ) <sub>4</sub> Na(W <sub>6</sub> O <sub>21+n</sub> H <sub>1+2n</sub> )•(8-n)H <sub>2</sub> O	0.9729	CdSeO <sub>4</sub> •2H <sub>2</sub> O
0.6935	AgNH <sub>2</sub> SO <sub>3</sub>	0.9741	FeAsO <sub>4</sub> •2H <sub>2</sub> O
0.7239	AgNO <sub>3</sub>	0.9751	FeP <sub>4</sub> O <sub>4</sub> •2H <sub>2</sub> O
0.7358	PdS <sub>2</sub>	0.9765	Cs <sub>2</sub> Se(SO <sub>3</sub> ) <sub>2</sub>
0.7428	Na <sub>2</sub> CO <sub>3</sub> •7H <sub>2</sub> O	0.9786	FeP <sub>4</sub> O <sub>4</sub> •2H <sub>2</sub> O
0.7622	Na <sub>2</sub> MoO <sub>4</sub> •2H <sub>2</sub> O	0.9836	InP <sub>4</sub> O <sub>4</sub> •2H <sub>2</sub> O
0.7627	PdSe <sub>2</sub>	0.9885	HgO <sub>2</sub>
0.7647	B <sub>8</sub> H <sub>12</sub>	0.9923	TlP <sub>4</sub> O <sub>4</sub> •2H <sub>2</sub> O
0.7716	Cu <sub>3</sub> (OH) <sub>3</sub> P <sub>4</sub>	0.9962	MnSeO <sub>4</sub> •2H <sub>2</sub> O
0.7722	Cu <sub>3</sub> (OH) <sub>3</sub> P <sub>4</sub>	0.9990	TlAsO <sub>4</sub> •2H <sub>2</sub> O

## Organic

0.1907	Ba(C <sub>8</sub> H <sub>12</sub> O <sub>3</sub> N) <sub>2</sub>	0.3980	NH <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> •OH
0.2143	NH <sub>2</sub> CH <sub>2</sub> (C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> ) <sub>4</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> CH <sub>3</sub> •HCl	0.4304	C <sub>6</sub> H <sub>4</sub> I <sub>2</sub>
0.2377	Cl <sub>3</sub> C•CH(C <sub>6</sub> H <sub>4</sub> SCH <sub>3</sub> ) <sub>2</sub>	0.4341	C <sub>6</sub> H <sub>4</sub> I <sub>2</sub>
0.2438	NH <sub>2</sub> CH <sub>2</sub> (C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> CH <sub>3</sub> •HCl	0.4364	(NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> C(OH)C <sub>6</sub> H <sub>3</sub> (CH <sub>3</sub> )NH <sub>2</sub>
0.2466	H <sub>2</sub> N(CH <sub>2</sub> ) <sub>8</sub> (CH <sub>2</sub> ) <sub>8</sub> CH <sub>2</sub> NH <sub>2</sub>	0.4369	C <sub>6</sub> H <sub>10</sub> (OH) <sub>2</sub>
0.2628	C <sub>10</sub> H <sub>6</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.4405	C <sub>8</sub> H <sub>10</sub> O <sub>2</sub>
0.2863	NH <sub>2</sub> CH <sub>2</sub> (C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> CH <sub>3</sub> •HBr	0.4441	C <sub>6</sub> H <sub>5</sub> COCH <sub>2</sub> CO <sub>2</sub> C <sub>6</sub> H <sub>5</sub>
0.2884	NH <sub>2</sub> CH <sub>2</sub> (C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> CH <sub>3</sub> •HCl	0.4467	P(CH <sub>3</sub> ) <sub>3</sub> -AuBr <sub>3</sub>
0.3053	C <sub>10</sub> H <sub>7</sub> •NH <sub>2</sub>	0.4501	C <sub>6</sub> H <sub>4</sub> (COOH)(CO <sub>2</sub> NH <sub>3</sub> CH <sub>3</sub> )
0.3083	C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>	0.4514	(ClC <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> C•C(CN) <sub>2</sub>
0.3227	C <sub>6</sub> H <sub>4</sub> (CO <sub>2</sub> CH <sub>3</sub> ) <sub>2</sub>	0.4538	CH <sub>3</sub> NH <sub>2</sub>
0.3236	C <sub>20</sub> H <sub>23</sub> IN <sub>2</sub> O <sub>4</sub>	0.4567	C <sub>6</sub> H <sub>5</sub> (CH:CH) <sub>5</sub> C <sub>6</sub> H <sub>5</sub>
0.3278	H <sub>6</sub> OC•CHF•CH <sub>2</sub> OH•CO <sub>2</sub> H	0.4737	C <sub>6</sub> H <sub>3</sub> (NO <sub>2</sub> ) <sub>3</sub>
0.3356	CH <sub>3</sub> (NH <sub>2</sub> ) <sub>6</sub> H <sub>3</sub> SO <sub>2</sub> NHC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	0.4764	C <sub>4</sub> H <sub>5</sub> SO <sub>2</sub> NH <sub>2</sub> •HCl
0.3510	(C <sub>2</sub> H <sub>5</sub> )(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> C <sub>2</sub> H <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	0.4787	C <sub>13</sub> H <sub>10</sub> O <sub>3</sub>
0.3527	Cu(C <sub>2</sub> H <sub>5</sub> NH <sub>3</sub> ) <sub>2</sub> Cl <sub>4</sub>	0.4814	(H <sub>2</sub> )C <sub>6</sub> H <sub>4</sub> CO <sub>2</sub> C <sub>6</sub> H <sub>5</sub>
0.3534	Fe(C <sub>5</sub> H <sub>4</sub> CO <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	0.4828	C <sub>8</sub> H <sub>9</sub> NO
0.3542	C <sub>2</sub> H <sub>5</sub> CO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> •C(C <sub>2</sub> H <sub>5</sub> ):C(C <sub>2</sub> H <sub>5</sub> )•C <sub>6</sub> H <sub>4</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	0.4886	Cl•C <sub>6</sub> H <sub>4</sub> •N:NPF <sub>6</sub>
0.3551	(C <sub>2</sub> H <sub>5</sub> )(C <sub>6</sub> H <sub>5</sub> ) <sub>5</sub> C <sub>5</sub> H <sub>5</sub> N <sub>2</sub> O <sub>2</sub> •H <sub>2</sub> O	0.4895	C <sub>12</sub> H <sub>9</sub> NO <sub>2</sub>
0.3603	(C <sub>6</sub> H <sub>5</sub> •C <sub>5</sub> H <sub>5</sub> )Co(C <sub>5</sub> H <sub>5</sub> )	0.4923	Cl•C <sub>6</sub> H <sub>4</sub> •N:NBF <sub>4</sub>
0.3603	NaS <sub>2</sub> CN(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	0.5008	CH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> •N:NBF <sub>4</sub>
0.3611	H <sub>2</sub> N(CH <sub>2</sub> ) <sub>6</sub> NH <sub>2</sub>	0.5050	C <sub>6</sub> H <sub>5</sub> (CH:CH) <sub>4</sub> C <sub>6</sub> H <sub>5</sub>
0.3619	Nl(SCS <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	0.5083	H <sub>3</sub> P <sub>4</sub> O <sub>4</sub> •OC(NH <sub>2</sub> ) <sub>2</sub>
0.3715	CH <sub>3</sub> -CO-NH-C <sub>6</sub> H <sub>4</sub> -CO-CH <sub>3</sub>	0.5112	C <sub>10</sub> H <sub>4</sub> Br <sub>2</sub> I <sub>2</sub>
0.3733	C <sub>12</sub> H <sub>12</sub>	0.5116	C <sub>19</sub> H <sub>12</sub> Br <sub>2</sub> N <sub>2</sub>
0.3780	C <sub>6</sub> H <sub>5</sub> CO•NHC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub>	0.5124	OC(NH <sub>2</sub> ) <sub>2</sub> •H <sub>3</sub> P <sub>4</sub> O <sub>4</sub>
0.3914	C <sub>6</sub> H <sub>4</sub> (CO <sub>2</sub> H)CO <sub>2</sub> NH <sub>4</sub>	0.5184	Co(NH <sub>3</sub> ) <sub>5</sub> Cl(ClO <sub>4</sub> )(CH <sub>3</sub> CO <sub>2</sub> )
0.3940	Hg(SCH <sub>3</sub> ) <sub>2</sub>	0.5221	CH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> •NO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> •O

Pbca D<sub>2h</sub><sup>15</sup> No. 61 (continued)

## Organic (continued)

0.5223	CH <sub>3</sub> COC <sub>6</sub> H <sub>4</sub> •C <sub>6</sub> H <sub>4</sub> I	0.7459	C <sub>4</sub> H <sub>5</sub> N $\theta$ <sub>2</sub>
0.5261	KAg(NCSe) <sub>2</sub>	0.7470	C <sub>2</sub> H <sub>4</sub> ( $\theta\theta$ C•C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
0.5281	C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> Ni $\theta$ <sub>2</sub>	0.7523	C <sub>22</sub> H <sub>14</sub>
0.5285	[(C <sub>5</sub> H <sub>5</sub> )Fe(C $\theta$ )] <sub>4</sub>	0.7564	Cu(C <sub>5</sub> $\theta$ <sub>5</sub> )•3H <sub>2</sub> $\theta$
0.5330	C <sub>16</sub> H <sub>14</sub>	0.7590	C <sub>10</sub> H <sub>15</sub> $\theta$ N•HCl
0.5337	[(H <sub>2</sub> N) <sub>2</sub> CS] <sub>2</sub> Cl <sub>2</sub>	0.7595	Ca(HC $\theta\theta$ ) <sub>2</sub>
0.5342	CH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> •N:NPF <sub>6</sub>	0.7610	Cd(HC $\theta\theta$ ) <sub>2</sub>
0.5398	(C $\theta$ Cl) <sub>2</sub>	0.7617	$\theta$ sHBr(C $\theta$ )[P(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> ] <sub>3</sub>
0.5420	CH <sub>3</sub> COC <sub>6</sub> H <sub>4</sub> •C <sub>6</sub> H <sub>4</sub> Br	0.7619	H $\theta$ C <sub>6</sub> H <sub>4</sub> •C(C:CHCH <sub>3</sub> )•C(C:CH•CH <sub>3</sub> )C <sub>6</sub> H <sub>4</sub> $\theta$ H
0.5493	C <sub>6</sub> H <sub>5</sub> (CH:CH) <sub>3</sub> C <sub>6</sub> H <sub>5</sub>	0.7621	C <sub>10</sub> H <sub>10</sub> PtCl <sub>2</sub>
0.5512	CH <sub>3</sub> $\theta$ •C <sub>6</sub> H <sub>4</sub> •CH:CBr•C $\theta\theta$ H	0.7635	C <sub>6</sub> H <sub>5</sub> •N:N•C <sub>6</sub> H <sub>4</sub> SBr
0.5543	C <sub>16</sub> H <sub>23</sub> N $\theta$ <sub>2</sub> •HBr	0.7686	( $\theta$ •C <sub>6</sub> H <sub>4</sub> •CH:NC <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> Ni
0.5606	(CH <sub>3</sub> ) <sub>2</sub> C <sub>7</sub> H <sub>5</sub> •C $\theta\theta$ CH <sub>2</sub> •C $\theta$ C <sub>6</sub> H <sub>4</sub> Br	0.7718	C <sub>6</sub> H <sub>6</sub>
0.5625	(H <sub>2</sub> N•C(NH)•NH•C(NH)•NH <sub>2</sub> ) <sub>2</sub> Se <sub>4</sub> •H <sub>2</sub> $\theta$	0.7722	MnC <sub>5</sub> $\theta$ <sub>5</sub> •3H <sub>2</sub> $\theta$
0.5682	C <sub>6</sub> H <sub>5</sub> C $\theta\theta$ •C $\theta$ C <sub>6</sub> H <sub>5</sub>	0.7791	(C <sub>6</sub> H <sub>5</sub> C•CC•CCu) <sub>2</sub> [P(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> ] <sub>3</sub>
0.5731	C <sub>13</sub> H <sub>20</sub> N $\theta$ <sub>2</sub> •HCl	0.7795	Zn(C <sub>5</sub> $\theta$ <sub>5</sub> )•3H <sub>2</sub> $\theta$
0.5741	S <sub>2</sub> (S <sub>2</sub> $\theta$ <sub>2</sub> C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.7818	H <sub>2</sub> NCN
0.5749	C <sub>16</sub> H <sub>20<math>\theta</math><sub>2</sub></sub>	0.7981	C <sub>30</sub> H <sub>46</sub> Cl <sub>2</sub> N $\theta$ <sub>6</sub>
0.5909	C(CH <sub>2</sub> $\theta$ CH) <sub>4</sub>	0.7993	NH <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> •S $\theta$ <sub>2</sub> NH <sub>2</sub>
0.5994	IrCl <sub>3</sub> •[(CH <sub>2</sub> ) <sub>2</sub> AsC <sub>6</sub> H <sub>4</sub> $\theta$ CH <sub>3</sub> ] <sub>3</sub>	0.8044	C <sub>2</sub> H <sub>5</sub> $\theta$ •C <sub>6</sub> H <sub>4</sub> •CH:C•C $\theta\theta$ H
0.6012	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> C <sub>3</sub> S <sub>3</sub>	0.8064	C <sub>6</sub> H <sub>5</sub> C•CCu•P(CH <sub>3</sub> ) <sub>3</sub>
0.6136	C <sub>6</sub> H <sub>5</sub> CH $\theta$ HC $\theta\theta$ H	0.8125	C <sub>20</sub> H <sub>19</sub> IN <sub>2</sub> S
0.6140	C <sub>14</sub> H <sub>14</sub> Cl <sub>6</sub> $\theta$ <sub>2</sub> S	0.8125	C <sub>2</sub> H <sub>6</sub> N <sub>4</sub> $\theta$ <sub>4</sub>
0.6156	H <sub>9</sub> H <sub>13</sub> NH(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	0.8236	(C <sub>4</sub> H <sub>5</sub> $\theta$ ) <sub>3</sub> CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CrCl <sub>2</sub>
0.6159	C <sub>6</sub> H <sub>5</sub> •CH:CBr•C $\theta\theta$ H	0.8291	N <sub>4</sub> S <sub>4</sub> (CH <sub>2</sub> $\theta$ H) <sub>4</sub>
0.6166	C <sub>9</sub> H <sub>7</sub> Cl $\theta$ <sub>4</sub> S <sub>2</sub>	0.8293	(C $\theta\theta$ H) <sub>2</sub>
0.6178	C <sub>9</sub> H <sub>7</sub> Cl $\theta$ <sub>4</sub> S <sub>2</sub>	0.8342	C <sub>2</sub> H <sub>2</sub> $\theta$ <sub>4</sub>
0.6216	C <sub>14</sub> H <sub>16</sub> P <sub>2</sub> S <sub>2</sub>	0.8405	C <sub>4</sub> H <sub>4</sub> (C <sub>3</sub> H <sub>2</sub> $\theta$ <sub>2</sub> ) <sub>2</sub>
0.6224	BaSe(S <sub>2</sub> $\theta$ <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> $\theta$ •C <sub>2</sub> H <sub>5</sub> $\theta$ H	0.8413	Cd[SC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> Se <sub>4</sub> •2H <sub>2</sub> $\theta$
0.6245	BaS(S <sub>2</sub> $\theta$ <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> $\theta$ •C <sub>2</sub> H <sub>5</sub> $\theta$ H	0.8421	C <sub>26</sub> H <sub>25</sub> NP <sub>2</sub> •PdCl <sub>2</sub>
0.6251	C <sub>10</sub> H <sub>10</sub> Cl <sub>2</sub> $\theta$ <sub>4</sub>	0.8424	C <sub>4</sub> NH <sub>2</sub> (NCS) <sub>2</sub> CH <sub>2</sub> •C <sub>6</sub> H <sub>5</sub>
0.6267	C <sub>9</sub> H <sub>13</sub> N $\theta$ <sub>2</sub>	0.8441	C <sub>10</sub> H <sub>7</sub> $\theta$ <sub>14</sub> N <sub>7</sub>
0.6268	Cu(N $\theta$ <sub>3</sub> ) <sub>2</sub> •(C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> ) <sub>2</sub>	0.8519	C <sub>16</sub> H <sub>21</sub> N $\theta$ <sub>3</sub> •HBr
0.6273	LiH <sub>2</sub> C $\theta$ <sub>2</sub> CH <sub>2</sub> C $\theta$ HC $\theta$ <sub>2</sub> CH <sub>2</sub> C $\theta$ <sub>2</sub> •H <sub>2</sub> $\theta$	0.8579	(C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>2</sub> [(CH <sub>3</sub> ) <sub>2</sub> C] <sub>4</sub> Ni(Cl $\theta$ <sub>4</sub> ) <sub>2</sub>
0.6308	Cu(HC $\theta\theta$ ) <sub>2</sub>	0.8588	C <sub>13</sub> H <sub>8</sub> $\theta$
0.6326	Nd(H <sub>2</sub> $\theta$ ) <sub>2</sub> N(C <sub>3</sub> H <sub>3</sub> C $\theta\theta$ ) <sub>3</sub> •H <sub>2</sub> $\theta$	0.8621	C <sub>16</sub> H <sub>32</sub> N <sub>4</sub> •Ni(Cl $\theta$ <sub>4</sub> ) <sub>2</sub>
0.6326	Te[(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> PS <sub>2</sub> ] <sub>2</sub>	0.8671	C <sub>15</sub> H <sub>17</sub> Br $\theta$ <sub>3</sub>
0.6383	N $\theta$ <sub>2</sub> •C <sub>6</sub> H <sub>4</sub> N:NBF <sub>4</sub>	0.8727	Cd[SC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> Se <sub>2</sub> •3H <sub>2</sub> $\theta$
0.6401	C <sub>9</sub> H <sub>8</sub> Cl <sub>6</sub> $\theta$ <sub>2</sub> S	0.8729	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub>
0.6408	(C <sub>14</sub> H <sub>10</sub> ) <sub>2</sub>	0.8750	CH <sub>3</sub> (C <sub>6</sub> H <sub>4</sub> )SC <sub>6</sub> H <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub>
0.6446	C <sub>6</sub> H <sub>10</sub> ( $\theta$ H) <sub>2</sub>	0.8776	Fe(CNCH <sub>3</sub> ) <sub>4</sub> (CN) <sub>2</sub>
0.6468	C <sub>17</sub> H <sub>19</sub> ClN <sub>2</sub> S	0.8809	C <sub>3</sub> H <sub>6</sub> N $\theta$ <sub>6</sub>
0.6480	[C <sub>6</sub> H <sub>4</sub> :(CH) <sub>2</sub> :C <sub>6</sub> H <sub>4</sub> ] <sub>2</sub>	0.8911	Cl•C <sub>6</sub> H <sub>4</sub> N:NBF <sub>4</sub>
0.6646	C <sub>5</sub> H <sub>2</sub> FN <sub>2</sub> $\theta$ <sub>4</sub> Rb•H <sub>2</sub> $\theta$	0.8912	N•C-C•N
0.6685	[Cu <sub>2</sub> (CH <sub>3</sub> C $\theta\theta$ ) <sub>4</sub> •(C <sub>5</sub> H <sub>5</sub> N) <sub>2</sub> ]	0.8933	HgCl <sub>2</sub> •(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> As $\theta$
0.6711	C <sub>8</sub> H <sub>8</sub> CuCl	0.8954	(CH <sub>3</sub> ) <sub>6</sub> C <sub>6</sub> Cr(C $\theta$ ) <sub>3</sub>
0.6718	S(CN) <sub>2</sub>	0.8972	CaC $\theta$ <sub>3</sub>
0.6724	C <sub>16</sub> H <sub>30</sub> $\theta$ <sub>4</sub> N <sub>3</sub> Br	0.8984	CaPd(CN) <sub>4</sub> •5H <sub>2</sub> $\theta$
0.6752	Cu(CH <sub>3</sub> C $\theta\theta$ ) <sub>2</sub> •C <sub>9</sub> H <sub>7</sub> N	0.8995	CaPt(CN) <sub>4</sub> •5H <sub>2</sub> $\theta$
0.6780	C <sub>16</sub> H <sub>30</sub> $\theta$ <sub>4</sub> N <sub>3</sub> Cl	0.8999	C <sub>6</sub> H <sub>10</sub> N $\theta$ <sub>2</sub>
0.6785	Na(H $\theta$ CH <sub>2</sub> S $\theta$ <sub>2</sub> )•2H <sub>2</sub> $\theta$	0.9039	N $\theta$ <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CH <sub>3</sub>
0.6803	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> S <sub>2</sub>	0.9043	C <sub>8</sub> H <sub>6</sub> N $\theta$ <sub>2</sub> •2H <sub>2</sub> $\theta$
0.6814	C <sub>6</sub> H <sub>2</sub> K $\theta$ <sub>2</sub> $\theta$ <sub>8</sub>	0.9121	C <sub>9</sub> H <sub>4</sub> $\theta$ <sub>3</sub>
0.6825	C <sub>14</sub> H <sub>10</sub> Cr(C $\theta$ ) <sub>3</sub>	0.9166	(C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> ) <sub>3</sub> Ni(Cl $\theta$ <sub>4</sub> ) <sub>2</sub>
0.6833	C <sub>10</sub> H <sub>4</sub> (N $\theta$ <sub>2</sub> ) <sub>4</sub>	0.9266	Te(C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> S) <sub>2</sub> Br <sub>4</sub>
0.6843	C <sub>10</sub> H <sub>9</sub> N $\theta$ <sub>3</sub> S	0.9271	N <sub>4</sub> P <sub>4</sub> ( $\theta$ CH <sub>3</sub> ) <sub>8</sub>
0.6918	C <sub>15</sub> H <sub>11</sub> N	0.9340	Fe(C <sub>5</sub> H <sub>7</sub> $\theta$ <sub>2</sub> ) <sub>3</sub>
0.6982	CH <sub>3</sub> C $\theta$ N(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>	0.9353	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> C <sub>3</sub> S <sub>2</sub> •SC <sub>2</sub> H <sub>5</sub> •I
0.6992	C <sub>10</sub> H <sub>8</sub> N $\theta$ <sub>3</sub> STl	0.9353	Fe(CH <sub>2</sub> C $\theta$ CH <sub>2</sub> C $\theta$ CH <sub>3</sub> ) <sub>3</sub>
0.7029	CH <sub>3</sub> •CN <sub>4</sub> •NHCH <sub>3</sub>	0.9387	NiBr <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> As(CH <sub>2</sub> ) <sub>3</sub> As•CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> As(CH <sub>3</sub> ) <sub>2</sub>
0.7036	C <sub>14</sub> H <sub>16</sub> N $\theta$ <sub>2</sub>	0.9410	Te(C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> S) <sub>2</sub> Cl <sub>4</sub>
0.7043	C(NH <sub>2</sub> ) <sub>3</sub> Cl	0.9532	Mo(C $\theta$ ) <sub>4</sub> •C <sub>6</sub> H <sub>4</sub> [As(CH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub>
0.7050	Cu(C <sub>10</sub> H <sub>12</sub> N $\theta$ ) <sub>2</sub>	0.9543	C <sub>18</sub> H <sub>22</sub> N $\theta$ <sub>2</sub> S•C <sub>4</sub> H <sub>4</sub> $\theta$ <sub>4</sub>
0.7111	(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> C <sub>4</sub> ClSNCl <sub>5</sub>	0.9617	NH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> F $\theta$ <sub>3</sub> H
0.7140	H <sub>2</sub> NCH <sub>2</sub> -CH <sub>2</sub> -C $\theta\theta$ H	0.9618	(CH <sub>3</sub> ) <sub>3</sub> NiCl
0.7184	(CH <sub>3</sub> ) <sub>2</sub> N•CHN <sub>4</sub>	0.9623	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> PC <sub>6</sub> H <sub>4</sub> Br
0.7227	C <sub>12</sub> H <sub>28</sub> N $\theta$ <sub>2</sub> Cl <sub>2</sub> •(C <sub>6</sub> H <sub>6</sub> N $\theta$ <sub>2</sub> ) <sub>4</sub>	0.9644	C <sub>8</sub> H <sub>6</sub> N $\theta$ <sub>2</sub> •2H <sub>2</sub> $\theta$
0.7255	C <sub>13</sub> H <sub>16</sub> $\theta$ <sub>3</sub>	0.9668	C <sub>9</sub> H <sub>18</sub> N $\theta$ <sub>2</sub> $\theta$ <sub>3</sub> •HBr
0.7259	C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> C $\theta\theta$ H	0.9680	C <sub>2</sub> H <sub>3</sub> N <sub>3</sub>
0.7263	C <sub>14</sub> H <sub>6</sub> $\theta$ <sub>2</sub> •P( $\theta$ C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub>	0.9714	C <sub>17</sub> H <sub>9</sub> $\theta$ Br
0.7320	ZnCl <sub>2</sub> •2NH <sub>2</sub> C $\theta$ N(CH <sub>3</sub> ) <sub>2</sub>	0.9722	(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> As•C <sub>9</sub> FN <sub>6</sub>
0.7326	NH <sub>2</sub> CH <sub>2</sub> C $\theta\theta$ CH <sub>2</sub> CH <sub>3</sub> •HCl	0.9746	Li[Fe(H <sub>2</sub> $\theta$ )( $\theta\theta$ CH <sub>2</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(CH <sub>2</sub> C $\theta\theta$ ) <sub>2</sub> ]•2H <sub>2</sub> $\theta$
0.7379	(C <sub>12</sub> H <sub>16</sub> N $\theta$ ) <sub>2</sub> Ni	0.9752	Cl <sub>2</sub> SeC <sub>4</sub> H <sub>8</sub> SeCl <sub>2</sub>
0.7428	K <sub>2</sub> C $\theta$ <sub>3</sub> •7H <sub>2</sub> $\theta$	0.9757	C <sub>6</sub> H <sub>4</sub> S <sub>2</sub>



Pbca  $D_{2h}^{15}$  No. 61 (continued)

Organic (continued)

0.9772	$(CH_3)_3C_6H_2 \cdot S_2 \cdot CH_3$	0.9896	$C_{19}H_{14}$
0.9827	$C_6H_5 \cdot C_6H_5 \cdot C_6H_5 \cdot C_6H_5 \cdot C_6H_5 \cdot C_6H_5$	0.9920	$(C_6H_5)_2C_3S_2 \cdot SCH_3 \cdot I$
0.9888	$(C_6H_5)_2SeCl_2$	0.9991	$Ru(NO)(S_2CN(C_2H_5)_2)_3$

 $\begin{matrix} 2 & 2 & 2 \\ m & m & m \end{matrix}$ Pnma  $D_{2h}^{16}$  No. 62Inorganic - 794  
Organic - 124

Inorganic

0.2746	$Mo_4O_{11}$	0.5110	$SrZn_5$
0.2812	$MoO_3$	0.5113	$K_2AgI_3$
0.2832	$IrSe_2$	0.5117	$(NH_4)_2AgI_3$
0.2860	$MoO_3$	0.5123	$C_2MoU$
0.2864	$MoO_3$	0.5136	$SrZnO_2$
0.3386	$Au_4Zr$	0.5150	$Rh_2AgI_3$
0.3433	$Ba_2Fe_2O_5$	0.5162	$BaCdO_2$
0.3462	$[(Cu, Pb)_5Bi_5S_{12}]$	0.5172	$Mn_3(PO_4)(BO_3) \cdot 3H_2O$
0.3497	$KTiNbO_5$	0.5179	$CsCr_3O_8$
0.3546	$FeNa_2(OH)(SO_4)_2 \cdot 3H_2O$	0.5208	$(V, Fe)O_2$
0.3589	$Zn_2P_2O_7 \cdot 4H_2O$	0.5341	$CrMoONi$
0.3638	$Sr_2Fe_2O_5$	0.5438	$SbCl_5 \cdot POCl_3$
0.3666	$Fe(OH)(SO_4) \cdot 2H_2O$	0.5441	$NbCl_5 \cdot POCl_3$
0.3732	$PbS$	0.5488	$TaCl_5 \cdot POCl_3$
0.3736	$PbSnS_2$	0.5496	$B_3Ni_4$
0.3745	$(HgCN)_2O$	0.5541	$Al_3(OH)_3(PO_4)_2 \cdot 5H_2O$
0.3775	$PbTe$	0.5546	$Al_3(OH)_3(PO_4)_2 \cdot 5H_2O$
0.3777	$PbSnS_2$	0.5617	$LiLaO_2$
0.3781	$PbSe$	0.5684	$BaSi_2O_5$
0.3786	$Ge_3Pt_2$	0.5720	$Al_{15}Nb_4S_{51}Ni_{10}$
0.3791	$[(Y, Er), U, Th](Nb, Ta, Ti, Fe)_2O_6$	0.5745	$CaMgSiO_4$
0.3823	$Ca_4Al_2Fe_2O_{10}$	0.5749	$CaMgSiO_4$
0.3842	$Ca_2Fe_2O_5$	0.5754	$BeCr_2O_4$
0.3848	$Ca_2FeAlO_5$	0.5760	$C_3Fe_7$
0.3855	$SnSe$	0.5767	$Ca(Fe, Mg, Mn)SiO_4$
0.3873	$SnS$	0.5778	$CaCoSiO_4$
0.3921	$(Y, Er)(Ti, Nb)_2O_6$	0.5782	$CsPbBr_3$
0.3949	$NiTh$	0.5783	$LiMgPO_4$
0.4059	$GeSe$	0.5784	$LiNaFeF_4$
0.4069	$GeSe$	0.5794	$AlFeBeO_4$
0.4087	$KClO_3$	0.5796	$AlGaBeO_4$
0.4117	$GeS$	0.5803	$(Fe, Mn)LiPO_4$
0.4156	$CuSbS_2$	0.5804	$CoLiPO_4$
0.4175	$CuSbSe_2$	0.5807	$Zn_3(PO_4)_2 \cdot 4H_2O$
0.4187	$CsIO_4$	0.5809	$C_3Mn_7$
0.4191	$CsReO_4$	0.5809	$CuFe_2S_3$
0.4221	$CuBiS_2$	0.5810	$Li_3CrO_4$
0.4257	$HMnO_2$	0.5811	$Fe_2SiO_4$
0.4320	$Cr(O_2)_2(NH_3)_3$	0.5812	$Li_3PO_4$
0.4356	$TlReO_4$	0.5816	$Mg_2SnS_4$
0.4531	$Cu_2O(FeO_3)$	0.5818	$CaMnSiO_4$
0.4554	$(V, Fe)O_6H$	0.5818	$Fe_2SiO_4$
0.4616	$FeO(OH)$	0.5818	$Mg_2GeS_4$
0.4664	$AlO(OH)$	0.5820	$Li(Mn, Fe)PO_4$
0.4667	$BaSe(S_2O_3)_2 \cdot 2H_2O$	0.5824	$FeLiPO_4$
0.4668	$SrSe(S_2O_3)_2 \cdot 2H_2O$	0.5825	$Al_2BeO_4$
0.4668	$LiSmO_2$	0.5825	$Mn_2GeS_4$
0.4671	$AlO(OH)$	0.5831	$Li_3AsO_4$
0.4671	$HgCl_2$	0.5832	$LiMnPO_4$
0.4677	$LiEuO_2$	0.5832	$LiNiPO_4$
0.4682	$HgCl_2$	0.5833	$Co_2SiO_4$
0.4691	$AlO(OH)$	0.5834	$(Al, Fe)_7BSi_3O_{18}$
0.4697	$LiGdO_2$	0.5835	$CaMnSiO_4$
0.4722	$LiTbO_2$	0.5837	$(Mg, Fe)_2SiO_4$
0.4729	$BaS(S_2O_3)_2 \cdot 2H_2O$	0.5837	$Li_3PO_4$
0.4733	$AlO(OH)$	0.5838	$Mg_2SiO_4$
0.4771	$K_2CuCl_2SO_4$	0.5844	$Ni_2SiO_4$
0.4785	$MnO_2$	0.5847	$Mg_2GeO_4$
0.4802	$CuAsS$	0.5848	$(Mg_{0.9}Fe_{0.1})_2SiO_4$
0.4817	$C_2Cr_3$	0.5848	$(Li, Na)_2(Fe, Mn)_5(PO_4)_4$
0.4890	$MnO_2$	0.5850	$Mn_2GeO_4$
0.4904	$Mg_5[Mg(F, OH)]_2(SiO_4)_3$	0.5858	$Mn_2SiO_4$
0.5009	$NaHgCl_3 \cdot 2H_2O$	0.5862	$(Mg, Fe)_2SiO_4$
0.5084	$V_2O_5$	0.5864	$Mn_2GeO_4$

Pnma  $D_{2h}^{16}$  No. 62 (continued)

## Inorganic (continued)

0.5864	Cu(N <sub>3</sub> ) <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub>	0.6779	Eu(Nb,Ti) <sub>2</sub> Si <sub>6</sub>
0.5869	Mn <sub>2</sub> SiS <sub>4</sub>	0.6781	(Ce,Ca)(Nb,Ti,Fe) <sub>2</sub> Si <sub>6</sub>
0.5869	Mg <sub>2</sub> SnSe <sub>4</sub>	0.6781	CaTa <sub>2</sub> Si <sub>6</sub>
0.5873	Mg <sub>2</sub> Si <sub>4</sub>	0.6785	GdNbTi <sub>6</sub>
0.5875	(Mg <sub>1-x</sub> Fe <sub>x</sub> ) <sub>2</sub> Si <sub>6</sub>	0.6798	Sm(Ta,Ti) <sub>2</sub> Si <sub>6</sub>
0.5876	Mg <sub>2</sub> Si <sub>4</sub>	0.6801	Sm(Nb,Ti) <sub>2</sub> Si <sub>6</sub>
0.5886	CaMgGe <sub>4</sub>	0.6803	EuNbTi <sub>6</sub>
0.5888	CaPbI <sub>3</sub>	0.6809	CaNaP <sub>4</sub>
0.5888	(Li,Mn)FeP <sub>4</sub>	0.6812	SmNbTi <sub>6</sub>
0.5900	(Mg,Fe) <sub>2</sub> Si <sub>4</sub>	0.6834	Nd(Nb,Ti) <sub>2</sub> Si <sub>6</sub>
0.5903	Cd <sub>2</sub> Ge <sub>4</sub>	0.6840	NdNbTi <sub>6</sub>
0.5904	Mn <sub>2</sub> Si <sub>4</sub>	0.6842	Nd(Ta,Ti) <sub>2</sub> Si <sub>6</sub>
0.5907	Mn <sub>2</sub> Si <sub>4</sub>	0.6854	Pr(Nb,Ti) <sub>2</sub> Si <sub>6</sub>
0.5908	Mg <sub>2</sub> SiSe <sub>4</sub>	0.6861	PrNbTi <sub>6</sub>
0.5910	Mg <sub>2</sub> SiS <sub>4</sub>	0.6867	Cu <sub>3</sub> (OH) <sub>4</sub> Si <sub>4</sub>
0.5939	Mn <sub>2</sub> SiSe <sub>4</sub>	0.6875	Ce(Nb,Ti) <sub>2</sub> Si <sub>6</sub>
0.5957	Ca <sub>2</sub> Ge <sub>4</sub>	0.6878	Ce(Ta,Ti) <sub>2</sub> Si <sub>6</sub>
0.5964	Ca <sub>2</sub> Si <sub>4</sub>	0.6879	CeNbTi <sub>6</sub>
0.5982	NaCo <sub>2</sub> .31(Mo <sub>4</sub> ) <sub>3</sub>	0.6893	K <sub>2</sub> Sn <sub>3</sub>
0.5990	Ca <sub>2</sub> SnS <sub>4</sub>	0.6901	ClF <sub>3</sub>
0.6000	Zr(OH) <sub>2</sub> Si <sub>4</sub>	0.6903	LaNbTi <sub>6</sub>
0.6000	Na <sub>3</sub> P <sub>3</sub> O <sub>9</sub>	0.6913	LaNbTi <sub>6</sub>
0.6001	KV <sub>3</sub> OH <sub>2</sub>	0.6918	Co <sub>2</sub> Si
0.6008	MnNaP <sub>4</sub>	0.6922	K <sub>2</sub> Ti <sub>3</sub>
0.6011	(Mn,Fe)P <sub>4</sub>	0.6925	LaTiTa <sub>6</sub>
0.6012	Ca <sub>2</sub> GeS <sub>4</sub>	0.6927	K <sub>2</sub> ReF <sub>8</sub>
0.6016	Th(OH) <sub>2</sub> Si <sub>4</sub>	0.6927	La(Ta,Ti) <sub>2</sub> Si <sub>6</sub>
0.6019	Na <sub>2</sub> BeF <sub>4</sub>	0.6930	NH <sub>4</sub> I <sub>3</sub>
0.6022	U(OH) <sub>2</sub> Si <sub>4</sub>	0.6937	La(Nb,Ti) <sub>2</sub> Si <sub>6</sub>
0.6029	Te <sub>2</sub> OH <sub>4</sub>	0.6940	TaI <sub>5</sub>
0.6030	KCdCl <sub>3</sub>	0.6953	HCl <sub>4</sub> •2H <sub>2</sub> O
0.6035	CdRbCl <sub>3</sub>	0.7006	Nb <sub>3</sub> Cl <sub>7</sub>
0.6040	NH <sub>4</sub> CdCl <sub>3</sub>	0.7016	NaAuCl <sub>4</sub> •2H <sub>2</sub> O
0.6054	Ca <sub>2</sub> Si <sub>4</sub>	0.7018	KN <sub>3</sub>
0.6064	Ca <sub>2</sub> SiS <sub>4</sub>	0.7026	KMnF <sub>3</sub>
0.6080	Mo <sub>4</sub> P <sub>3</sub>	0.7058	K <sub>2</sub> RuCl <sub>5</sub> •H <sub>2</sub> O
0.6080	Ca <sub>2</sub> SiSe <sub>4</sub>	0.7069	K <sub>4</sub> [Mo(CN) <sub>8</sub> ]•2H <sub>2</sub> O
0.6118	S <sub>7</sub> NH	0.7074	Ca <sub>2</sub> TaV <sub>6</sub>
0.6130	S <sub>6</sub> (NH) <sub>2</sub>	0.7074	CeCr <sub>3</sub>
0.6189	Sr(OH) <sub>2</sub>	0.7078	LaFe <sub>3</sub>
0.6213	Cu(OH)I <sub>3</sub>	0.7079	SmAl <sub>3</sub>
0.6218	Al <sub>3</sub> Ca <sub>2</sub> (OH)(Si <sub>4</sub> ) <sub>3</sub>	0.7091	Ca <sub>2</sub> NbV <sub>6</sub>
0.6248	Sn <sub>2</sub> S <sub>3</sub>	0.7092	LaB <sub>3</sub>
0.6260	Ca <sub>2</sub> Al <sub>3</sub> (OH)(Si <sub>2</sub> OH)(Si <sub>4</sub> ) <sub>3</sub>	0.7092	CaV <sub>3</sub>
0.6288	S <sub>5</sub> N <sub>3</sub> H <sub>3</sub>	0.7094	NdB <sub>3</sub>
0.6320	Cu(NH <sub>3</sub> ) <sub>2</sub> (SCN) <sub>2</sub>	0.7094	LaGa <sub>3</sub>
0.6365	PBr <sub>7</sub>	0.7096	EuAl <sub>3</sub>
0.6445	Na <sub>3</sub> P <sub>3</sub> O <sub>9</sub> •H <sub>2</sub> O	0.7098	Ni <sub>2</sub> Si
0.6471	NiS <sub>2</sub> •6H <sub>2</sub> O	0.7103	NdCr <sub>3</sub>
0.6490	MgS <sub>2</sub> •6H <sub>2</sub> O	0.7105	SrZr <sub>3</sub>
0.6510	MgS <sub>2</sub> •6H <sub>2</sub> O	0.7110	LaCr <sub>3</sub>
0.6513	TlHgCl <sub>3</sub>	0.7110	PrGa <sub>3</sub>
0.6566	S <sub>4</sub> N <sub>4</sub> H <sub>4</sub>	0.7113	PrCr <sub>3</sub>
0.6620	TlHgBr <sub>3</sub>	0.7116	LaB <sub>3</sub>
0.6647	Pb <sub>6</sub> St <sub>2</sub> S <sub>9</sub>	0.7122	CaTi <sub>3</sub>
0.6667	[Ru(NH <sub>3</sub> ) <sub>4</sub> S <sub>2</sub> Cl]Cl	0.7122	GdAl <sub>3</sub>
0.6706	LuNbTi <sub>6</sub>	0.7123	LaSi
0.6709	YbNbTi <sub>6</sub>	0.7139	SiTb
0.6718	CaFe <sub>2</sub> FeOH(Si <sub>4</sub> ) <sub>2</sub>	0.7140	(Ca,Na)(Nb,Ti,Fe) <sub>3</sub>
0.6718	TmNbTi <sub>6</sub>	0.7140	NdCr <sub>3</sub>
0.6736	Dy(Ta,Ti) <sub>2</sub> Si <sub>6</sub>	0.7140	NdGa <sub>3</sub>
0.6737	ErNbTi <sub>6</sub>	0.7142	PrFe <sub>3</sub>
0.6754	K <sub>2</sub> Zr <sub>3</sub>	0.7146	LaSc <sub>3</sub>
0.6755	YNbTi <sub>6</sub>	0.7147	PrV <sub>3</sub>
0.6755	[Y(Nb,Ti) <sub>2</sub> Si <sub>6</sub> ]	0.7156	(PNF <sub>2</sub> ) <sub>3</sub>
0.6759	YTi <sub>1.5</sub> W <sub>0.5</sub> Si <sub>6</sub>	0.7160	EuC <sub>3</sub>
0.6765	GdTi <sub>1.5</sub> W <sub>0.5</sub> Si <sub>6</sub>	0.7163	GdSi
0.6767	GdTITa <sub>6</sub>	0.7165	PrSi
0.6769	CaFe <sub>2</sub> FeOH(Si <sub>4</sub> ) <sub>2</sub>	0.7168	K <sub>2</sub> S <sub>3</sub> Si <sub>6</sub>
0.6769	Gd(Ta,Ti) <sub>2</sub> Si <sub>6</sub>	0.7169	MgNaF <sub>3</sub>
0.6771	YTiSb <sub>6</sub>	0.7169	SrU <sub>3</sub>
0.6773	DyNbTi <sub>6</sub>	0.7170	DyAl <sub>3</sub>
0.6776	TbNbTi <sub>6</sub>	0.7171	SiSm
0.6776	GdTISb <sub>6</sub>	0.7171	NaNiF <sub>3</sub>

Pnma  $D_{2h}^{16}$  No. 62 (continued)

## Inorganic (continued)

0.7174	NdSi	0.7346	K <sub>2</sub> BeF <sub>4</sub>
0.7174	SrUO <sub>3</sub>	0.7348	DyFeO <sub>3</sub>
0.7179	DySi	0.7349	YGaO <sub>3</sub>
0.7180	SrCeO <sub>3</sub>	0.7350	ErFeO <sub>3</sub>
0.7184	CeSi	0.7352	TmFeO <sub>3</sub>
0.7184	PrSi	0.7353	(NH <sub>4</sub> ) <sub>2</sub> BeF <sub>4</sub>
0.7185	SmCrO <sub>3</sub>	0.7353	ErFeO <sub>3</sub>
0.7186	GeRh <sub>2</sub>	0.7354	LuCrO <sub>3</sub>
0.7188	NdFeO <sub>3</sub>	0.7355	HoFeO <sub>3</sub>
0.7189	LaRhO <sub>3</sub>	0.7356	YbCrO <sub>3</sub>
0.7190	CaZrO <sub>3</sub>	0.7356	YbGaO <sub>3</sub>
0.7192	SmCrO <sub>3</sub>	0.7357	Tl <sub>2</sub> S <sub>6</sub>
0.7196	PrScO <sub>3</sub>	0.7358	YFeO <sub>3</sub>
0.7196	NdFeO <sub>3</sub>	0.7362	GdVO <sub>3</sub>
0.7197	CeSi	0.7363	Tl <sub>2</sub> BeF <sub>4</sub>
0.7201	CaUO <sub>3</sub>	0.7374	BFe
0.7202	SiTb	0.7376	BFe
0.7204	ErSi	0.7377	Pb(OH)Br
0.7204	CaCO <sub>3</sub>	0.7379	SiU
0.7205	SiSm	0.7385	NdRhO <sub>3</sub>
0.7206	LaInO <sub>3</sub>	0.7387	Cs <sub>2</sub> TlCl <sub>5</sub> •H <sub>2</sub> O
0.7209	HoSi	0.7391	Ge <sub>2</sub> Mo
0.7209	(NH <sub>4</sub> ) <sub>2</sub> BeF <sub>4</sub>	0.7391	Ni <sub>2</sub> (OH) <sub>3</sub> Cl
0.7210	LaSi	0.7397	K <sub>2</sub> S <sub>6</sub>
0.7211	NdSi	0.7407	(NH <sub>4</sub> ) <sub>2</sub> MnF <sub>5</sub>
0.7211	GeLa	0.7416	TbCrO <sub>3</sub>
0.7214	HoSi	0.7424	K <sub>2</sub> P <sub>3</sub> F
0.7216	CoLa <sub>3</sub>	0.7427	P <sub>2</sub> Zr
0.7216	NdScO <sub>3</sub>	0.7434	As <sub>2</sub> SiO <sub>4</sub>
0.7217	K <sub>2</sub> FeCl <sub>5</sub> •H <sub>2</sub> O	0.7440	K <sub>2</sub> S <sub>6</sub>
0.7222	CeGe	0.7441	Co(NH <sub>3</sub> ) <sub>5</sub> ClI <sub>2</sub>
0.7222	(NH <sub>4</sub> ) <sub>2</sub> FeCl <sub>5</sub> •H <sub>2</sub> O	0.7449	CoSeO <sub>4</sub>
0.7224	GePr	0.7451	BTl
0.7224	(Pb, Ca)CO <sub>3</sub>	0.7455	BMn
0.7226	DySi	0.7455	SmRhO <sub>3</sub>
0.7227	NdVO <sub>3</sub>	0.7458	Rb <sub>2</sub> CrO <sub>4</sub>
0.7229	PbCO <sub>3</sub>	0.7460	CuSeO <sub>4</sub>
0.7231	Pb(OH) <sub>2</sub>	0.7461	GdRhO <sub>3</sub>
0.7231	LaRhO <sub>3</sub>	0.7466	Pb(OH)I
0.7236	YScO <sub>3</sub>	0.7468	LiCN
0.7236	EuCrO <sub>3</sub>	0.7475	SiTh
0.7237	BaCO <sub>3</sub>	0.7475	Mn <sub>2</sub> (OH) <sub>3</sub> Cl
0.7237	SrCO <sub>3</sub>	0.7476	Mg <sub>2</sub> (OH) <sub>3</sub> Cl
0.7245	GdCrO <sub>3</sub>	0.7480	HfP <sub>2</sub>
0.7252	SmFeO <sub>3</sub>	0.7486	Rb <sub>2</sub> S <sub>6</sub>
0.7254	NdInO <sub>3</sub>	0.7487	P <sub>2</sub> Ti
0.7261	Tl <sub>2</sub> SeO <sub>4</sub>	0.7488	Mn <sub>2</sub> (OH) <sub>3</sub> Br
0.7263	GdScO <sub>3</sub>	0.7489	MgSeO <sub>4</sub>
0.7271	YAlO <sub>3</sub>	0.7492	Cu <sub>2</sub> (OH) <sub>3</sub> Cl
0.7280	GdGaO <sub>3</sub>	0.7505	Cu <sub>2</sub> (OH) <sub>3</sub> Cl
0.7283	SmInO <sub>3</sub>	0.7506	Cs <sub>2</sub> CoCl <sub>4</sub>
0.7285	BRh <sub>2</sub>	0.7506	Cs <sub>2</sub> ZnCl <sub>4</sub>
0.7300	EuFeO <sub>3</sub>	0.7510	Cs <sub>2</sub> CrO <sub>4</sub>
0.7303	Tl <sub>2</sub> CrO <sub>4</sub>	0.7517	Sr <sub>2</sub> SiO <sub>4</sub>
0.7304	PrRhO <sub>3</sub>	0.7525	CFe <sub>3</sub>
0.7308	K <sub>2</sub> SeO <sub>4</sub>	0.7527	Cs <sub>2</sub> S <sub>6</sub>
0.7309	DyCrO <sub>3</sub>	0.7530	BCo
0.7317	K <sub>2</sub> CrO <sub>4</sub>	0.7534	As <sub>2</sub> Zr
0.7318	YCrO <sub>3</sub>	0.7536	ErRhO <sub>3</sub>
0.7320	Pb(OH)Cl	0.7538	ZnSeO <sub>4</sub>
0.7321	Tl <sub>2</sub> S <sub>6</sub>	0.7543	Se(SeCN) <sub>2</sub>
0.7322	HoCrO <sub>3</sub>	0.7543	Cs <sub>2</sub> ZnBr <sub>4</sub>
0.7324	GdFeO <sub>3</sub>	0.7543	HoRhO <sub>3</sub>
0.7325	Rh <sub>2</sub> Si	0.7548	BHf
0.7326	(NH <sub>4</sub> ) <sub>2</sub> S <sub>6</sub>	0.7548	CFe <sub>3</sub>
0.7328	CaNaPO <sub>4</sub>	0.7550	KNp <sub>2</sub> F <sub>9</sub>
0.7332	LuFeO <sub>3</sub>	0.7555	KPu <sub>2</sub> F <sub>9</sub>
0.7334	Np	0.7560	U(SO <sub>4</sub> ) <sub>2</sub> •4H <sub>2</sub> O
0.7336	ErCrO <sub>3</sub>	0.7562	Rb <sub>2</sub> BeF <sub>4</sub>
0.7337	ThFeO <sub>3</sub>	0.7563	K <sub>2</sub> WS <sub>4</sub>
0.7341	YbFeO <sub>3</sub>	0.7573	As <sub>2</sub> Hf
0.7341	LaMnO <sub>3</sub>	0.7573	KU <sub>2</sub> F <sub>9</sub>
0.7344	TmCrO <sub>3</sub>	0.7585	K <sub>2</sub> SnCl <sub>4</sub> •H <sub>2</sub> O
0.7344	DyFeO <sub>3</sub>	0.7591	Pd <sub>3</sub> Si

Pnma  $D_{2h}^{16}$  No. 62 (continued)

## Inorganic (continued)

0.7616	KTh <sub>2</sub> F <sub>9</sub>	0.8020	PPd <sub>3</sub>
0.7636	SiTi	0.8029	CuTaS <sub>3</sub>
0.7672	K <sub>2</sub> HgCl <sub>4</sub> •H <sub>2</sub> O	0.8046	LuPt
0.7678	(NH <sub>4</sub> ) <sub>2</sub> HgCl <sub>4</sub> •H <sub>2</sub> O	0.8046	MnPb(OH)(VO <sub>4</sub> )
0.7679	DyPt	0.8053	Pb(Zn,Cu)(OH)VO <sub>4</sub>
0.7691	MnSeO <sub>4</sub>	0.8056	BaSO <sub>4</sub>
0.7701	K <sub>2</sub> RuNOCl <sub>5</sub>	0.8057	BaMnO <sub>4</sub>
0.7709	NiY	0.8060	BaCrO <sub>4</sub>
0.7715	K <sub>2</sub> MoS <sub>4</sub>	0.8064	CsAg <sub>2</sub> I <sub>3</sub>
0.7721	(NH <sub>4</sub> ) <sub>2</sub> WS <sub>4</sub>	0.8065	BaCrO <sub>4</sub>
0.7729	BaKPO <sub>4</sub>	0.8065	Y <sub>2</sub> Pt <sub>3</sub> (CN) <sub>12</sub> •21H <sub>2</sub> O
0.7734	ErNi	0.8068	BaSO <sub>4</sub>
0.7740	DyNi	0.8074	NH <sub>4</sub> ClO <sub>4</sub>
0.7744	[Co(NH <sub>3</sub> ) <sub>5</sub> Cl]Cl <sub>2</sub>	0.8076	SrBr <sub>2</sub> •H <sub>2</sub> O
0.7746	NiTm	0.8078	PdTh
0.7751	P <sub>4</sub> S <sub>3</sub>	0.8086	SnSO <sub>4</sub>
0.7757	Rb <sub>2</sub> WS <sub>4</sub>	0.8087	Mg <sub>3</sub> (SO <sub>4</sub> )(B <sub>2</sub> O <sub>5</sub> )•5H <sub>2</sub> O
0.7760	Rb <sub>2</sub> MoS <sub>4</sub>	0.8088	PbMnOHVO <sub>4</sub>
0.7760	LuNi	0.8096	HClO <sub>4</sub> •H <sub>2</sub> O
0.7764	DyNi	0.8098	NH <sub>4</sub> ClO <sub>4</sub>
0.7779	F <sub>2</sub> O <sub>5</sub>	0.8102	FeSb <sub>2</sub> S <sub>4</sub>
0.7779	CoSO <sub>4</sub>	0.8112	CsBF <sub>4</sub>
0.7781	GdPt	0.8117	CuSO <sub>4</sub>
0.7786	CoSO <sub>4</sub>	0.8119	BaBr <sub>2</sub> •H <sub>2</sub> O
0.7801	BiSCL	0.8120	Er <sub>2</sub> Pt <sub>3</sub> (CN) <sub>12</sub> •21H <sub>2</sub> O
0.7803	(NH <sub>4</sub> ) <sub>3</sub> ZnCl <sub>5</sub>	0.8123	RbClO <sub>4</sub>
0.7812	MgSO <sub>4</sub>	0.8124	NH <sub>4</sub> MnO <sub>4</sub>
0.7812	(NH <sub>4</sub> ) <sub>2</sub> MoS <sub>4</sub>	0.8128	PbSO <sub>4</sub>
0.7812	PrPt	0.8137	SbSeBr
0.7813	BiSeBr	0.8151	BaSeO <sub>4</sub>
0.7813	Co(NH <sub>3</sub> ) <sub>5</sub> Cl <sub>3</sub>	0.8152	KMnO <sub>4</sub>
0.7814	TlBF <sub>4</sub>	0.8155	BaBOF <sub>3</sub>
0.7821	NdPt	0.8165	BaSeO <sub>4</sub>
0.7823	Rh(NH <sub>3</sub> ) <sub>5</sub> Cl <sub>3</sub>	0.8182	SrSO <sub>4</sub>
0.7823	Cs <sub>2</sub> WS <sub>4</sub>	0.8191	K <sub>2</sub> S <sub>6</sub> N <sub>2</sub>
0.7831	GdNi	0.8193	KClO <sub>4</sub>
0.7834	Bi <sub>3</sub> Rh	0.8198	KBF <sub>4</sub>
0.7844	ZnSO <sub>4</sub>	0.8201	PbSO <sub>4</sub>
0.7855	NaIO <sub>3</sub>	0.8207	PbSO <sub>4</sub>
0.7856	Cs <sub>2</sub> MoS <sub>4</sub>	0.8224	PbCrO <sub>4</sub>
0.7865	Cs <sub>2</sub> CuCl <sub>4</sub>	0.8224	CuPbOHAsO <sub>4</sub>
0.7866	PtSm	0.8234	EuSO <sub>4</sub>
0.7873	BNi <sub>3</sub>	0.8251	(MoO <sub>2</sub> ) <sub>2</sub> P <sub>2</sub> O <sub>7</sub>
0.7881	CsCuBr <sub>4</sub>	0.8264	BiSeI
0.7882	BCo <sub>3</sub>	0.8268	BiSBr
0.7887	GdPt	0.8296	(Mn,Pb) <sub>2</sub> (OH)VO <sub>4</sub>
0.7892	Na <sub>2</sub> H <sub>2</sub> P <sub>4</sub> O <sub>12</sub>	0.8297	PbSeO <sub>4</sub>
0.7892	CsMnO <sub>4</sub>	0.8305	BBO <sub>2</sub>
0.7896	BNi <sub>3</sub>	0.8306	BaTm <sub>2</sub> S <sub>4</sub>
0.7905	SiZr	0.8310	BaLu <sub>2</sub> S <sub>4</sub>
0.7910	S <sub>3</sub> (CN) <sub>2</sub>	0.8310	BaSm <sub>2</sub> S <sub>4</sub>
0.7912	CsMnO <sub>4</sub>	0.8310	P <sub>14</sub> PbZn
0.7920	PtY	0.8311	BaYb <sub>2</sub> S <sub>4</sub>
0.7924	PtTb	0.8311	SrLu <sub>2</sub> S <sub>4</sub>
0.7933	CsClO <sub>4</sub>	0.8315	BaEr <sub>2</sub> S <sub>4</sub>
0.7939	DyPt	0.8315	BaNd <sub>2</sub> S <sub>4</sub>
0.7944	Pb <sub>2</sub> Bi <sub>2</sub> S <sub>5</sub>	0.8322	BaSm <sub>2</sub> Se <sub>4</sub>
0.7948	CeCu <sub>6</sub>	0.8323	SrYb <sub>2</sub> S <sub>4</sub>
0.7958	(Ba,Sr)SO <sub>4</sub>	0.8326	Pb <sub>3</sub> Bi <sub>2</sub> S <sub>6</sub>
0.7959	HoPt	0.8326	SrEr <sub>2</sub> S <sub>4</sub>
0.7962	TlClO <sub>4</sub>	0.8327	SrTm <sub>2</sub> S <sub>4</sub>
0.7971	RbBF <sub>4</sub>	0.8328	RbSe <sub>3</sub> F
0.7974	CuSO <sub>4</sub>	0.8328	NH <sub>4</sub> Se <sub>3</sub> F
0.7980	NH <sub>4</sub> BF <sub>4</sub>	0.8332	SrHo <sub>2</sub> S <sub>4</sub>
0.7981	FPd <sub>3</sub>	0.8333	SbSeI
0.7983	CeCu <sub>6</sub>	0.8334	BaGd <sub>2</sub> S <sub>4</sub>
0.7983	PtTm	0.8334	SrDy <sub>2</sub> S <sub>4</sub>
0.7984	ErPt	0.8334	SrTb <sub>2</sub> S <sub>4</sub>
0.7999	LiClO <sub>4</sub>	0.8335	BiSi
0.8000	BaCl <sub>2</sub> •H <sub>2</sub> O	0.8335	TlF <sub>3</sub>
0.8008	Pb <sub>3</sub> O <sub>2</sub> Br <sub>2</sub>	0.8338	BaDy <sub>2</sub> S <sub>4</sub>
0.8010	RbMnO <sub>4</sub>	0.8340	Ca <sub>2</sub> Sn
0.8013	[N <sub>3</sub> Co(NH <sub>3</sub> ) <sub>5</sub> ](N <sub>3</sub> ) <sub>2</sub>	0.8341	BaHO <sub>2</sub> S <sub>4</sub>
0.8020	BaFeO <sub>4</sub>	0.8342	BaI <sub>2</sub>

Pnma  $D_{2h}^{16}$  No. 62 (continued)

## Inorganic (continued)

0.8344	BaBr <sub>2</sub>	0.8616	CaSc <sub>2</sub> Cl <sub>4</sub>
0.8347	SrY <sub>2</sub> S <sub>4</sub>	0.8617	Ca <sub>2</sub> Si
0.8348	SrSm <sub>2</sub> Cl <sub>4</sub>	0.8622	CaFe <sub>2</sub> Cl <sub>4</sub>
0.8348	BaCl <sub>2</sub>	0.8630	CaV <sub>2</sub> Cl <sub>4</sub>
0.8348	HgCl	0.8634	K <sub>3</sub> VS <sub>4</sub>
0.8350	SrTb <sub>2</sub> Se <sub>4</sub>	0.8641	AsCo
0.8352	BaY <sub>2</sub> S <sub>4</sub>	0.8642	CaFe <sub>2</sub> Cl <sub>4</sub>
0.8352	BF <sub>3</sub> •2H <sub>2</sub> O	0.8658	K <sub>3</sub> PS <sub>4</sub>
0.8357	BaTb <sub>2</sub> S <sub>4</sub>	0.8667	SrH <sub>2</sub>
0.8363	CdP <sub>14</sub> Pb	0.8670	BaH <sub>2</sub>
0.8364	Eu <sub>3</sub> Cl <sub>4</sub>	0.8673	Co(NCl) <sub>2</sub> Cl
0.8367	Eu <sub>3</sub> Cl <sub>4</sub>	0.8673	YbD <sub>2</sub>
0.8367	BaCl <sub>2</sub>	0.8673	EuD <sub>2</sub>
0.8367	Ca <sub>2</sub> Pb	0.8676	AsCo
0.8367	HgP <sub>14</sub> Pb	0.8681	CaH <sub>2</sub>
0.8371	SrDy <sub>2</sub> Se <sub>4</sub>	0.8685	(NH <sub>4</sub> ) <sub>3</sub> AsS <sub>4</sub>
0.8382	BaGd <sub>2</sub> Se <sub>4</sub>	0.8710	FePTi
0.8382	BaCl <sub>2</sub>	0.8711	(NH <sub>4</sub> ) <sub>3</sub> VS <sub>4</sub>
0.8384	BaBr <sub>2</sub>	0.8712	CeCu
0.8387	BaI <sub>2</sub>	0.8730	CoPTa
0.8388	Eu <sub>2</sub> SrCl <sub>4</sub>	0.8731	CsI <sub>2</sub> Er
0.8388	SrGd <sub>2</sub> Cl <sub>4</sub>	0.8733	(NSCl) <sub>3</sub>
0.8390	As <sub>2</sub> Pb <sub>5</sub> Sb <sub>6</sub> S <sub>15</sub>	0.8743	FePTa
0.8394	SrY <sub>2</sub> Se <sub>4</sub>	0.8759	CoNbP
0.8394	SmCl <sub>2</sub>	0.8762	FeNbP
0.8396	ThSe <sub>2</sub>	0.8762	NiSiTi
0.8404	SrDy <sub>2</sub> Cl <sub>4</sub>	0.8779	CrP
0.8404	US <sub>2</sub>	0.8781	MgSc <sub>2</sub> Cl <sub>4</sub>
0.8406	SbSI	0.8783	CoPTi
0.8413	EuCl <sub>2</sub>	0.8784	HgS <sub>4</sub> •H <sub>2</sub> O
0.8422	PbF <sub>2</sub>	0.8796	GeRh
0.8424	BaY <sub>2</sub> Se <sub>4</sub>	0.8797	FePZr
0.8425	BaDy <sub>2</sub> Se <sub>4</sub>	0.8824	AsMn
0.8425	PhCl <sub>2</sub>	0.8844	CoPZr
0.8427	SrEr <sub>2</sub> Se <sub>4</sub>	0.8860	IrSi
0.8429	ThS <sub>2</sub>	0.8885	MnP
0.8433	SrNd <sub>2</sub> Cl <sub>4</sub>	0.8889	MnP
0.8437	SbSBr	0.8910	CrP
0.8441	SrEr <sub>2</sub> Cl <sub>4</sub>	0.8928	NH <sub>4</sub> I <sub>3</sub>
0.8444	SrHo <sub>2</sub> Cl <sub>4</sub>	0.8934	GeIr
0.8445	PbBr <sub>2</sub>	0.8954	FeP
0.8454	SbSBr	0.8962	FeP
0.8455	BaSm <sub>2</sub> Cl <sub>4</sub>	0.8975	Al <sub>3</sub> Ni
0.8458	SrTb <sub>2</sub> Cl <sub>4</sub>	0.8999	CsI <sub>3</sub>
0.8466	BaEr <sub>2</sub> Se <sub>4</sub>	0.9020	PRu
0.8467	SnCl <sub>2</sub>	0.9023	AsFe
0.8473	BaYb <sub>2</sub> Se <sub>4</sub>	0.9042	Ca <sub>2</sub> Y <sub>2</sub> (Si <sub>4</sub> Cl <sub>12</sub> )(Cl <sub>3</sub> )•H <sub>2</sub> O
0.8477	SrYb <sub>2</sub> Se <sub>4</sub>	0.9066	CoP
0.8480	BaPr <sub>2</sub> Cl <sub>4</sub>	0.9087	CoP
0.8485	SrLu <sub>2</sub> Cl <sub>4</sub>	0.9102	LuF <sub>3</sub>
0.8494	SrLu <sub>2</sub> Se <sub>4</sub>	0.9106	AsCr
0.8495	BaLu <sub>2</sub> Se <sub>4</sub>	0.9107	Ca <sub>2</sub> (RE) <sub>2</sub> Si <sub>4</sub> Cl <sub>12</sub> (Cl <sub>3</sub> )•H <sub>2</sub> O
0.8496	SrTm <sub>2</sub> Cl <sub>4</sub>	0.9129	PdSi
0.8499	CaSc <sub>2</sub> Cl <sub>4</sub>	0.9154	CaB <sub>2</sub> Si <sub>2</sub> Cl <sub>8</sub>
0.8507	Fe <sub>3</sub> BCl <sub>6</sub>	0.9160	YbF <sub>3</sub>
0.8509	SrYb <sub>2</sub> Cl <sub>4</sub>	0.9168	CaB <sub>2</sub> Si <sub>2</sub> Cl <sub>8</sub>
0.8513	Al <sub>3</sub> Mn	0.9202	P <sub>3</sub> N <sub>3</sub> Cl <sub>6</sub>
0.8520	TlBr <sub>3</sub> •4H <sub>2</sub> O	0.9212	PW
0.8528	Ca <sub>2</sub> Ge	0.9217	NiSi
0.8529	Cs <sub>2</sub> Re <sub>3</sub> Br <sub>11</sub>	0.9217	NH <sub>4</sub> NCl <sub>3</sub>
0.8542	Co <sub>2</sub> P	0.9225	TmF <sub>3</sub>
0.8549	CaCr <sub>2</sub> Cl <sub>4</sub>	0.9238	GePd
0.8549	Mg <sub>3</sub> (F,OH) <sub>2</sub> Si <sub>4</sub> Cl <sub>4</sub>	0.9258	N <sub>3</sub> P <sub>3</sub> Br <sub>6</sub>
0.8551	NH <sub>4</sub> ClBrI	0.9260	GeNi
0.8559	PRu <sub>2</sub>	0.9281	ErF <sub>3</sub>
0.8559	HNCl <sub>3</sub> •3S <sub>8</sub>	0.9294	YF <sub>3</sub>
0.8570	F <sub>3</sub> Rh <sub>4</sub>	0.9294	CaU <sub>6</sub> Cl <sub>19</sub> •10-11H <sub>2</sub> O
0.8574	SbCl <sub>3</sub>	0.9295	TlReCl <sub>3</sub> S
0.8581	SrSc <sub>2</sub> Cl <sub>4</sub>	0.9300	NaBeSi <sub>3</sub> Cl <sub>7</sub> (OH)
0.8588	KS <sub>3</sub> F	0.9315	HoF <sub>3</sub>
0.8598	NiPTa	0.9318	BIF <sub>3</sub>
0.8609	TlCl <sub>3</sub> •4H <sub>2</sub> O	0.9333	AsMo
0.8612	CsIBr <sub>2</sub>	0.9333	NH <sub>4</sub> NCl <sub>3</sub>
0.8614	NbNiP	0.9354	DyF <sub>3</sub>

Prma D<sub>2h</sub><sup>16</sup> No. 62 (continued)

## Inorganic (continued)

0.9357	(NH <sub>4</sub> ) <sub>2</sub> CuBr <sub>3</sub>	0.9700	BiCuPbS <sub>3</sub>
0.9373	TbF <sub>3</sub>	0.9717	Np <sub>2</sub> S <sub>3</sub>
0.9393	RhSb	0.9721	Ce <sub>3</sub> UO <sub>2</sub> (NCS) <sub>5</sub>
0.9407	GdF <sub>3</sub>	0.9735	(Mg, Fe) <sub>3</sub> TiB <sub>2</sub> O <sub>8</sub>
0.9413	KBF <sub>4</sub>	0.9739	(Mg, Fe) <sub>7</sub> H <sub>2</sub> (SiO <sub>3</sub> ) <sub>8</sub>
0.9417	GePt	0.9742	Fe <sub>6</sub> HSO <sub>4</sub>
0.9432	PtSi	0.9755	Al <sub>2</sub> SiO <sub>5</sub>
0.9434	EuF <sub>3</sub>	0.9758	(Mg, Fe, Mn, Al) <sub>7</sub> (Si, Al) <sub>8</sub> O <sub>22</sub> (OH) <sub>2</sub>
0.9448	SmF <sub>3</sub>	0.9763	Fe <sub>2</sub> Fe <sub>2</sub> B <sub>2</sub> O <sub>8</sub>
0.9459	Ni(NH <sub>3</sub> ) <sub>3</sub> (NCS) <sub>2</sub>	0.9774	U <sub>2</sub> S <sub>3</sub>
0.9492	Ce <sub>2</sub> AgI <sub>3</sub>	0.9775	Fe <sub>2</sub> Ni <sub>2</sub> B <sub>2</sub> O <sub>8</sub>
0.9497	KPt <sub>2</sub> F <sub>2</sub>	0.9796	AuGa
0.9498	LiBH <sub>4</sub>	0.9801	In <sub>2</sub> Se <sub>3</sub>
0.9504	Sb <sub>4</sub> S <sub>5</sub> Cl <sub>2</sub>	0.9802	Dy <sub>2</sub> Se <sub>3</sub>
0.9526	Ba <sub>2</sub> ZnS <sub>3</sub>	0.9802	Al <sub>2</sub> SiO <sub>5</sub>
0.9539	Al <sub>2</sub> (F, OH) <sub>2</sub> SiO <sub>4</sub>	0.9806	Pu <sub>2</sub> Se <sub>3</sub>
0.9546	In <sub>6</sub> HSO <sub>4</sub>	0.9811	Nd <sub>2</sub> Te <sub>3</sub>
0.9547	(Mg, Fe, Mn, Al) <sub>7</sub> (Si, Al) <sub>8</sub> O <sub>22</sub> (OH) <sub>2</sub>	0.9820	PaH <sub>10</sub> (NH <sub>3</sub> ) <sub>2</sub>
0.9548	Al <sub>2</sub> SiO <sub>4</sub> (F, OH) <sub>2</sub>	0.9821	Mg <sub>2</sub> Fe <sub>2</sub> B <sub>2</sub> O <sub>8</sub>
0.9562	K <sub>2</sub> CuCl <sub>3</sub>	0.9821	Gd <sub>2</sub> Se <sub>3</sub>
0.9583	KAlGeO <sub>8</sub>	0.9824	Gd <sub>2</sub> Te <sub>3</sub>
0.9596	(Mg, Fe, Mn, Al) <sub>7</sub> (Si, Al) <sub>8</sub> O <sub>22</sub> (OH) <sub>2</sub>	0.9832	MgBTiO <sub>4</sub>
0.9600	Ce <sub>2</sub> AgCl <sub>3</sub>	0.9834	Sm <sub>2</sub> Te <sub>3</sub>
0.9607	(Mg, Fe, Mn, Al) <sub>7</sub> (Si, Al) <sub>8</sub> O <sub>22</sub> (OH) <sub>2</sub>	0.9838	Tb <sub>2</sub> Se <sub>3</sub>
0.9608	V <sub>6</sub> SO <sub>4</sub>	0.9843	Co <sub>2</sub> Fe <sub>2</sub> B <sub>2</sub> O <sub>8</sub>
0.9621	(Fe, Mg) <sub>5</sub> Al <sub>2</sub> (Si, Al) <sub>8</sub> O <sub>22</sub> (OH) <sub>2</sub>	0.9852	MgBV <sub>6</sub> O <sub>4</sub>
0.9648	La <sub>2</sub> TiO <sub>5</sub>	0.9872	Th <sub>2</sub> S <sub>3</sub>
0.9655	(Mg, Fe, Mn, Al) <sub>7</sub> (Si, Al) <sub>8</sub> O <sub>22</sub> (OH) <sub>2</sub>	0.9873	Sb <sub>2</sub> Se <sub>3</sub>
0.9667	Li <sub>2</sub> (Mg, Fe) <sub>3</sub> (Al, Fe) <sub>2</sub> Si <sub>8</sub> O <sub>22</sub> (OH) <sub>2</sub>	0.9876	Bi <sub>2</sub> S <sub>3</sub>
0.9669	Pb <sub>3</sub> U <sub>6</sub> O <sub>27</sub> •5H <sub>2</sub> O	0.9879	Na <sub>2</sub> S <sub>2</sub> O <sub>6</sub> •2H <sub>2</sub> O
0.9671	(NH <sub>4</sub> ) <sub>3</sub> Cl <sub>3</sub>	0.9887	Bi <sub>2</sub> (S, Se) <sub>3</sub>
0.9676	Mg <sub>7</sub> (Si <sub>4</sub> O <sub>11</sub> ) <sub>2</sub> (OH, F) <sub>2</sub>	0.9889	Sb <sub>2</sub> Se <sub>3</sub>
0.9677	NH <sub>4</sub> N <sub>3</sub>	0.9891	Al <sub>2</sub> O <sub>3</sub>
0.9678	Mg <sub>7</sub> Si <sub>8</sub> O <sub>22</sub> (OH) <sub>2</sub>	0.9900	(NH <sub>4</sub> ) <sub>2</sub> (UO <sub>2</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> •5H <sub>2</sub> O
0.9693	Al <sub>2</sub> Fe <sub>5</sub> Si <sub>6</sub> Al <sub>2</sub> O <sub>22</sub> (OH) <sub>2</sub>	0.9918	Y <sub>4</sub> Al <sub>2</sub> O <sub>9</sub>
0.9695	(Mg, Fe) <sub>7</sub> (OH) <sub>2</sub> Si <sub>8</sub> O <sub>22</sub>	0.9929	Sb <sub>2</sub> S <sub>3</sub>
0.9699	PdSn	1.0000	2NH <sub>3</sub> •H <sub>2</sub> O

## Organic

0.0913	C <sub>30</sub> H <sub>62</sub>	0.6229	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> S
0.2398	CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> •HgCl	0.6283	BaCl <sub>2</sub> [CH <sub>2</sub> (NH <sub>2</sub> )C(OH)] <sub>2</sub> •H <sub>2</sub> O
0.2541	C <sub>2</sub> H <sub>5</sub> •ZnI	0.6307	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> •HBr
0.3131	C <sub>9</sub> H <sub>7</sub> BrS <sub>2</sub>	0.6320	Cu(NH <sub>3</sub> ) <sub>2</sub> (SCN) <sub>2</sub>
0.3236	C <sub>6</sub> H <sub>5</sub> •C <sub>3</sub> H <sub>2</sub> S <sub>2</sub> Cl•H <sub>2</sub> O	0.6329	Nd <sub>2</sub> (C <sub>5</sub> H <sub>4</sub> N) <sub>2</sub>
0.3289	C <sub>9</sub> H <sub>7</sub> IS <sub>2</sub>	0.6499	CrO <sub>2</sub> (O <sub>2</sub> ) <sub>2</sub> •C <sub>12</sub> H <sub>8</sub> N <sub>2</sub>
0.3400	C <sub>6</sub> H <sub>5</sub> C <sub>3</sub> H <sub>2</sub> S <sub>2</sub> •SCN	0.6505	(C <sub>5</sub> H <sub>5</sub> FeS) <sub>4</sub>
0.3720	(H <sub>6</sub> OC•CH <sub>2</sub> ) <sub>2</sub> S	0.6514	C <sub>3</sub> H <sub>5</sub> IN <sub>2</sub> S <sub>2</sub>
0.3745	(HgCN) <sub>2</sub> O	0.6609	S <sub>2</sub> (C:NH) <sub>2</sub> NH•HI
0.3881	C <sub>7</sub> H <sub>8</sub> S <sub>3</sub>	0.6662	CnH <sub>2</sub> nO <sub>2</sub>
0.3884	CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	0.6688	Cu(N <sub>3</sub> ) <sub>2</sub> •CH <sub>3</sub> N <sub>2</sub> O
0.3999	CH <sub>3</sub> SO <sub>2</sub> SN <sub>2</sub> •H <sub>2</sub> O	0.6694	CnH <sub>2</sub> nO <sub>2</sub>
0.4052	C <sub>12</sub> H <sub>8</sub> N	0.6755	[Ni•NO <sub>2</sub> •(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> ]ClO <sub>4</sub>
0.4272	C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> )(C <sub>6</sub> H <sub>3</sub> )	0.680	(CH <sub>3</sub> O•C <sub>6</sub> H <sub>4</sub> •N:N)FeCl <sub>4</sub>
0.4475	C <sub>13</sub> H <sub>10</sub>	0.6803	C <sub>5</sub> H <sub>7</sub> N <sub>3</sub> O•HBr
0.4518	CH <sub>12</sub> BrCoN <sub>4</sub> O <sub>3</sub>	0.6805	Ni(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub> •NO <sub>2</sub> •BF <sub>4</sub>
0.4639	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	0.6851	(CCL <sub>3</sub> CH <sub>2</sub> ) <sub>3</sub>
0.4817	Cr <sub>3</sub> C <sub>2</sub>	0.6978	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub> •2H <sub>2</sub> O
0.5078	(CH <sub>2</sub> ) <sub>5</sub> N <sub>2</sub> (CH <sub>3</sub> ) <sub>6</sub> I <sub>2</sub> •0.25H <sub>2</sub> O	0.7018	Ru(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub>
0.5123	MoUC <sub>2</sub>	0.7069	K <sub>4</sub> [Mo(CN) <sub>8</sub> ]•2H <sub>2</sub> O
0.5321	SbCl <sub>5</sub> •PF <sub>6</sub> (CH <sub>3</sub> ) <sub>3</sub>	0.7117	NH <sub>3</sub> •C <sub>6</sub> H <sub>4</sub> •SO <sub>3</sub>
0.5333	(CH <sub>3</sub> ) <sub>3</sub> N <sub>2</sub> O•HCl	0.7160	EuCO <sub>3</sub>
0.5433	C <sub>3</sub> H <sub>6</sub> S <sub>3</sub>	0.7167	C <sub>8</sub> H <sub>8</sub> •Fe <sub>2</sub> (CO) <sub>5</sub>
0.5504	[(NH <sub>2</sub> ) <sub>2</sub> CNHC <sub>3</sub> ]N <sub>2</sub> O <sub>3</sub>	0.7204	CaCO <sub>3</sub>
0.5603	C <sub>5</sub> H <sub>4</sub> NC(OH)HCl	0.7224	(Pb, Ca)CO <sub>3</sub>
0.5667	N(CH <sub>3</sub> ) <sub>4</sub> Ag <sub>2</sub> I <sub>3</sub>	0.7229	PbCO <sub>3</sub>
0.5682	(CH <sub>3</sub> ) <sub>3</sub> SeI	0.7237	NH <sub>2</sub> C <sub>6</sub> NHCH <sub>3</sub> HN <sub>2</sub> O <sub>3</sub>
0.5735	(C <sub>10</sub> H <sub>7</sub> NH <sub>2</sub> )[Cr(NCS) <sub>4</sub> (NH <sub>3</sub> ) <sub>2</sub> ]	0.7237	BaCO <sub>3</sub>
0.5760	Fe <sub>7</sub> C <sub>3</sub>	0.7237	SrCO <sub>3</sub>
0.5809	Mn <sub>7</sub> C <sub>3</sub>	0.7251	(CH <sub>3</sub> ) <sub>2</sub> B <sub>5</sub> H <sub>7</sub>
0.5848	(C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> ) <sub>2</sub> S•I <sub>2</sub>	0.7335	(CH <sub>3</sub> ) <sub>3</sub> N•I <sub>2</sub>
0.5957	C <sub>6</sub> H <sub>3</sub> (OH) <sub>3</sub> •2H <sub>2</sub> O	0.7337	CH <sub>3</sub> SC <sub>2</sub> NH <sub>2</sub>
0.6048	Be(CO) <sub>2</sub> •3H <sub>2</sub> O	0.7370	[S <sub>2</sub> Fe <sub>3</sub> (CO) <sub>9</sub> ][S <sub>2</sub> Fe <sub>2</sub> (CO) <sub>6</sub> ]
0.6223	C <sub>6</sub> H <sub>5</sub> N <sub>2</sub> Cu <sub>2</sub> Br <sub>3</sub>	0.7468	LiCN

Pnma  $D_{2h}^{16}$  No. 62 (continued)

## Organic (continued)

0.7525	Fe <sub>3</sub> C	0.8692	C <sub>5</sub> H <sub>5</sub> Nb(C $\theta$ ) <sub>4</sub>
0.7534	CH <sub>3</sub> C $\theta$ NHCH <sub>3</sub>	0.8700	Al(BH <sub>4</sub> ) <sub>3</sub> $\theta$ (CH <sub>3</sub> ) <sub>3</sub> N
0.7543	Se(SeCN) <sub>2</sub>	0.8720	C <sub>2</sub> H <sub>5</sub> N <sub>5</sub>
0.7548	Fe <sub>3</sub> C	0.8760	C <sub>3</sub> H <sub>7</sub> N <sub>5</sub> $\theta$ HBr
0.7569	W(C <sub>6</sub> H <sub>6</sub> ) <sub>2</sub>	0.8806	C <sub>2</sub> Cl <sub>6</sub>
0.7614	K <sub>2</sub> [IrBr <sub>5</sub> (C $\theta$ )]	0.8807	C <sub>3</sub> H <sub>7</sub> N <sub>5</sub> $\theta$ HCl
0.7664	Mo(C <sub>6</sub> H <sub>6</sub> ) <sub>2</sub>	0.8812	C <sub>10</sub> H <sub>12</sub> $\theta$ <sub>4</sub>
0.7710	Zn[S(C(NH <sub>2</sub> )) <sub>2</sub> NHNH <sub>2</sub> ] <sub>2</sub> Cl <sub>2</sub>	0.8867	C <sub>2</sub> Br <sub>6</sub>
0.7825	ZnCl <sub>2</sub> $\theta$ 2(CH <sub>3</sub> $\theta$ CN)	0.8872	C <sub>2</sub> Cl <sub>3</sub> Br <sub>3</sub>
0.7881	CHCl <sub>3</sub>	0.8915	Cl <sub>3</sub> C-CCLBr <sub>2</sub>
0.7907	[N(CH <sub>3</sub> ) <sub>4</sub> ] <sub>2</sub> ZnCl <sub>4</sub>	0.8924	C <sub>2</sub> Br <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>
0.7910	S <sub>3</sub> (CN) <sub>2</sub>	0.8945	(C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> N $\theta$ ReBr <sub>4</sub> $\theta$ H <sub>2</sub> $\theta$
0.7953	[N(CH <sub>3</sub> ) <sub>4</sub> ] <sub>2</sub> CoCl <sub>4</sub>	0.8967	NH <sub>2</sub> CSNH <sub>2</sub>
0.8002	[N(CH <sub>3</sub> ) <sub>4</sub> ] <sub>2</sub> CuCl <sub>4</sub>	0.9030	(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> TiCl <sub>2</sub> Al(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>
0.8046	C <sub>7</sub> H <sub>9</sub> PdCl <sub>2</sub>	0.9080	C <sub>2</sub> Br <sub>5</sub> F
0.8046	SeC(NH <sub>2</sub> ) <sub>2</sub>	0.9305	C <sub>2</sub> H <sub>3</sub> N-BF <sub>3</sub>
0.8065	Y <sub>2</sub> Pt <sub>3</sub> (CN) <sub>12</sub> $\theta$ 21H <sub>2</sub> $\theta$	0.9320	C <sub>2</sub> Br <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>
0.8120	Er <sub>2</sub> Pt <sub>3</sub> (CN) <sub>12</sub> $\theta$ 21H <sub>2</sub> $\theta$	0.9459	Ni(NH <sub>3</sub> ) <sub>3</sub> (NCS) <sub>2</sub>
0.8144	H <sub>3</sub> CCN-BBr <sub>3</sub>	0.9470	Mo <sub>3</sub> $\theta$ <sub>4</sub> (C <sub>5</sub> H <sub>7</sub> $\theta$ <sub>2</sub> ) <sub>3</sub> (C <sub>2</sub> H <sub>5</sub> $\theta$ ) <sub>3</sub>
0.8411	(C <sub>5</sub> H <sub>5</sub> N)(CH <sub>3</sub> ) <sub>3</sub> SnCl	0.9510	(H <sub>2</sub> N) <sub>2</sub> CS $\theta$ <sub>2</sub>
0.8450	(CH <sub>3</sub> ) <sub>3</sub> SnF	0.9569	C <sub>4</sub> H <sub>6</sub> Fe(C $\theta$ ) <sub>3</sub>
0.8479	(C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> As $\theta$ CuI	0.9612	C(NH <sub>2</sub> ) <sub>3</sub> Br
0.8480	[(CH <sub>3</sub> ) <sub>2</sub> PBH <sub>2</sub> ] <sub>3</sub>	0.9697	Cl <sub>2</sub> ErC-CBrCl <sub>2</sub>
0.8504	(BH <sub>2</sub> ) <sub>3</sub> (N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>3</sub>	0.9721	Cs <sub>3</sub> U $\theta$ <sub>2</sub> (NCS) <sub>5</sub>
0.8549	H <sub>3</sub> CCN-BCl <sub>3</sub>	0.9737	[(NH <sub>2</sub> ) <sub>2</sub> CS] <sub>2</sub> ZnCl <sub>2</sub>
0.8551	(C <sub>8</sub> H <sub>8</sub> )Fe(C $\theta$ ) <sub>3</sub>	0.9807	(C <sub>5</sub> H <sub>5</sub> )(C <sub>7</sub> H <sub>7</sub> )IV
0.8619	C <sub>3</sub> H <sub>7</sub> ClN <sub>2</sub>	0.9880	(ClC <sub>6</sub> H <sub>4</sub> ) <sub>3</sub> C <sub>3</sub> N <sub>3</sub>
0.8676	C <sub>5</sub> H <sub>5</sub> CoS <sub>2</sub> C <sub>4</sub> F <sub>6</sub>	0.9896	CH <sub>3</sub> CN $\theta$ 2HCl

 $\frac{2}{m} \frac{2}{m} \frac{2}{m}$ Cmcm  $D_{2h}^{17}$  No. 63Inorganic - 258  
Organic - 19

## Inorganic

0.1686	NdTe <sub>3</sub>	0.3330	GaI <sub>3</sub>
0.1687	TmTe <sub>3</sub>	0.3525	Rb $\theta$ H
0.1688	ErTe <sub>3</sub>	0.3535	K $\theta$ H
0.1688	DyTe <sub>3</sub>	0.3606	RuTh
0.1688	YTe <sub>3</sub>	0.3670	BMo
0.1689	HoTe <sub>3</sub>	0.3690	Tl <sub>2</sub> Ge <sub>6</sub> $\theta$ <sub>13</sub>
0.1689	TbTe <sub>3</sub>	0.3754	RhTh
0.1690	SmTe <sub>3</sub>	0.3778	BCr
0.1690	PrTe <sub>3</sub>	0.3779	CeRh
0.1690	LaTe <sub>3</sub>	0.3790	BCr
0.1691	GdTe <sub>3</sub>	0.3798	BW
0.1692	CeTe <sub>3</sub>	0.3806	AlY
0.1779	BCMo <sub>2</sub>	0.3809	LaRh
0.2297	AlBMo	0.3817	InBr
0.2497	Ge <sub>2</sub> Th	0.3824	CoTh
0.2527	HfSi <sub>12</sub>	0.3833	IrTh
0.2530	Ge <sub>2</sub> Zr	0.3848	InI
0.2546	Si <sub>2</sub> Zr	0.3859	PrRh
0.2567	Ge <sub>2</sub> Hf	0.3860	AlTh
0.2614	Ge <sub>2</sub> Sc	0.3899	Ga
0.2631	Si <sub>2</sub> Ti	0.3918	NdRh
0.2655	(Al, Si) <sub>2</sub> Ti	0.3926	AlZr
0.2689	Sn <sub>2</sub> Y	0.3941	GaSc
0.2698	GdSn <sub>2</sub>	0.3961	GaY
0.2702	Sn <sub>2</sub> Tb	0.3970	ErGe
0.2704	HoSn <sub>2</sub>	0.3972	GaTb
0.2705	DySn <sub>2</sub>	0.3985	GeY
0.2706	ErSn <sub>2</sub>	0.3989	ErGe
0.2713	Sn <sub>2</sub> Tm	0.3991	GeHo
0.2715	LuSn <sub>2</sub>	0.3993	DyGe
0.2728	Sb <sub>2</sub> Yb	0.3995	GeHo
0.2728	Ge <sub>2</sub> U	0.4001	DyGe
0.2758	Mo <sub>4</sub> $\theta$ <sub>10</sub> ( $\theta$ H) <sub>2</sub>	0.4005	GeSc
0.3001	Na $\theta$ H	0.4010	ENi
0.3016	Al $\theta$ ( $\theta$ H)	0.4012	GeTb
0.3041	Al $\theta$ ( $\theta$ H)	0.4015	GeSm
0.3059	Al $\theta$ ( $\theta$ H)	0.4016	PtTh
0.3082	Sc $\theta$ $\theta$ H	0.4018	GdGe
0.3088	Fe $\theta$ ( $\theta$ H)	0.4022	GdGe

Cmcm  $D_{2h}^{17}$  No. 63 (continued)

## Inorganic (continued)

0.4028	GeSm	0.7071	AmI <sub>3</sub>
0.4029	ErSi	0.7093	NpI <sub>3</sub>
0.4034	GeNd	0.7116	NdI <sub>3</sub>
0.4036	ScSi	0.7123	PrI <sub>3</sub>
0.4038	DySi	0.7128	LaI <sub>3</sub>
0.4039	SiY	0.7140	PuI <sub>3</sub>
0.4039	SiTm	0.7146	UI <sub>3</sub>
0.4041	GePr	0.7154	GeI <sub>3</sub>
0.4041	GeNd	0.7166	LaI <sub>3</sub>
0.4043	ErSi	0.7170	Nb <sub>12</sub> O <sub>29</sub>
0.4048	SiYb	0.7179	SbBr <sub>3</sub>
0.4053	LuSi	0.7196	Ti <sub>2</sub> Nb <sub>10</sub> O <sub>29</sub>
0.4054	HoSi	0.7207	CmBr <sub>3</sub>
0.4056	TlI	0.7222	AmBr <sub>3</sub>
0.4103	NiZrH <sub>3</sub>	0.7233	NpBr <sub>3</sub>
0.4105	LaNi	0.7235	PuBr <sub>3</sub>
0.4107	GdNi	0.7242	TbCl <sub>3</sub>
0.4112	NiTb	0.7245	NdBr <sub>3</sub>
0.4118	NiZr	0.7263	GdCl <sub>3</sub>
0.4128	NiZr	0.7282	CrVO <sub>4</sub>
0.4129	NiSm	0.7380	LiCr <sub>3</sub> O <sub>8</sub>
0.4130	LaPt	0.7400	CaIrO <sub>3</sub>
0.4132	CeNi	0.7419	ZnCrO <sub>4</sub>
0.4133	NiPu	0.7438	NiCrO <sub>4</sub>
0.4140	NiPr	0.7495	CoCrO <sub>4</sub>
0.4143	CePt	0.7516	C <sub>2</sub> Cr <sub>2</sub> V
0.4146	PtZr	0.7540	Hf <sub>4</sub> Cr <sub>7</sub>
0.4154	NdNi	0.7562	MgCrO <sub>4</sub>
0.4176	HfPt	0.7709	Na <sub>2</sub> CrO <sub>4</sub>
0.4178	CeNi	0.7731	CuSeO <sub>4</sub>
0.4185	CaSn	0.7736	Al <sub>2</sub> CuMg
0.4196	HfNi	0.7739	Te <sub>6</sub> O <sub>11</sub> Cl <sub>2</sub>
0.4198	BaPb	0.7790	Na <sub>2</sub> SO <sub>4</sub>
0.4219	CaGe	0.7793	ERe <sub>3</sub>
0.4225	EuGe	0.7829	BaZn <sub>5</sub>
0.4233	EuSi	0.7864	CrPO <sub>4</sub>
0.4252	CaSi	0.7882	NiSeO <sub>4</sub>
0.4263	SiSr	0.7910	ETc <sub>3</sub>
0.4435	BaFe <sub>2</sub> O <sub>4</sub>	0.7947	CdCrO <sub>4</sub>
0.4500	PbBiO <sub>2</sub> Cl	0.7985	HF
0.4529	PbBiO <sub>2</sub> Cl	0.7988	CsCu <sub>2</sub> Cl <sub>3</sub>
0.4574	PbSbO <sub>2</sub> Cl	0.8010	MgSeO <sub>4</sub>
0.4583	PbSbO <sub>2</sub> Cl	0.8052	CoSeO <sub>4</sub>
0.4619	Cs <sub>2</sub> RuCl <sub>5</sub> H <sub>2</sub> O	0.8082	NiSO <sub>4</sub>
0.4723	Ca <sub>2</sub> Mn <sub>3</sub> Si <sub>3</sub> O <sub>12</sub> (OH)	0.8120	ZnSeO <sub>4</sub>
0.4729	(Co, Ni) <sub>2</sub> MgFeSi <sub>8</sub> (Al, Fe) <sub>18</sub> O <sub>47</sub>	0.8166	BIPd
0.4730	Au <sub>3</sub> Mg	0.8191	Tl <sub>2</sub> AlF <sub>5</sub>
0.4734	Fe(OH) <sub>2</sub> Al <sub>4</sub> Si <sub>2</sub> O <sub>10</sub>	0.8243	MgSO <sub>4</sub>
0.4748	K <sub>2</sub> SbF <sub>5</sub>	0.8263	FeSO <sub>4</sub>
0.4762	(NH <sub>4</sub> ) <sub>2</sub> SbF <sub>5</sub>	0.8286	CoSO <sub>4</sub>
0.4776	Tl <sub>2</sub> SbF <sub>5</sub>	0.8292	CoSO <sub>4</sub>
0.4785	SrVO <sub>4</sub> Si <sub>2</sub> O <sub>6</sub>	0.8313	MnSeO <sub>4</sub>
0.4859	Rb <sub>2</sub> SbF <sub>5</sub>	0.8335	AgCuS
0.4913	Cs <sub>2</sub> SbF <sub>5</sub>	0.8344	Al <sub>5</sub> Fe <sub>2</sub>
0.4962	KPtBr <sub>3</sub> NH <sub>3</sub>	0.8361	Ca <sub>4</sub> (BeOH) <sub>2+x</sub> Al <sub>2-x</sub> Si <sub>9</sub> O <sub>26-x</sub>
0.4963	Cu(OH) <sub>2</sub>	0.8415	K <sub>5</sub> ThF <sub>9</sub>
0.5034	KPtCl <sub>3</sub> NH <sub>3</sub>	0.8431	U
0.5182	Na <sub>3</sub> (TiF <sub>6</sub> )(HF <sub>2</sub> )	0.8437	Al <sub>6</sub> Re
0.5252	Al <sub>60</sub> Mn <sub>11</sub> Ni <sub>4</sub>	0.8442	U
0.5294	AlMnZn	0.8478	Al <sub>6</sub> Te
0.5358	HgI <sub>2</sub>	0.8482	ZnCS <sub>3</sub> (NH <sub>3</sub> ) <sub>2</sub>
0.5457	Ag <sub>2</sub> CN	0.8514	Al <sub>6</sub> Mn
0.5985	KI·Hg(CN) <sub>2</sub>	0.8515	MnSO <sub>4</sub>
0.6021	BaSe(SO <sub>3</sub> ) <sub>2</sub> ·2H <sub>2</sub> O	0.8619	InPO <sub>4</sub>
0.6043	K <sub>2</sub> HfF <sub>6</sub>	0.8825	K <sub>2</sub> AlF <sub>5</sub> ·H <sub>2</sub> O
0.6102	K <sub>2</sub> ZrF <sub>6</sub>	0.8828	TlPO <sub>4</sub>
0.6182	Rh <sub>3</sub> Te <sub>2</sub>	0.9034	Pb(UO <sub>2</sub> ) <sub>4</sub> (OH) <sub>4</sub> (PO <sub>4</sub> ) <sub>2</sub> ·7H <sub>2</sub> O
0.6228	BaNiO <sub>2</sub>	0.9099	Ca(UO <sub>2</sub> ) <sub>4</sub> (OH) <sub>4</sub> (PO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O
0.6586	CuCrO <sub>4</sub>	0.9153	Ba(UO <sub>2</sub> ) <sub>4</sub> (OH) <sub>4</sub> (PO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O
0.6694	Al <sub>2</sub> Ca(Si <sub>2</sub> O <sub>7</sub> )(OH) <sub>2</sub> ·H <sub>2</sub> O	0.9611	Cu <sub>3</sub> Ti
0.6844	Na <sub>2</sub> Te·5H <sub>2</sub> O	0.9669	Al <sub>2</sub> TiO <sub>5</sub>
0.6899	Na <sub>2</sub> Se·5H <sub>2</sub> O	0.9740	CaTi <sub>2</sub> O <sub>4</sub>
0.6923	Na <sub>2</sub> Se·5H <sub>2</sub> O	0.9743	Ti <sub>3</sub> O <sub>5</sub>
0.7071	PuI <sub>3</sub>	0.9750	CaTi <sub>2</sub> O <sub>4</sub>



Cmcm  $D_{2h}^{17}$  No. 63 (continued)

## Inorganic (continued)

0.9759	AlB <sub>10</sub>	0.9913	MgDy <sub>2</sub> S <sub>4</sub>
0.9773	AgCd	0.9914	MnDy <sub>2</sub> S <sub>4</sub>
0.9780	Al <sub>2</sub> Ti <sub>5</sub>	0.9927	NaBF <sub>4</sub>
0.9800	MgTi <sub>2</sub> S <sub>5</sub>	0.9956	Na(BF <sub>3</sub> OH)
0.9859	Fe <sub>2</sub> Ti <sub>5</sub>	0.9969	Al <sub>2</sub> Ti <sub>5</sub>
0.9883	NaBF <sub>4</sub>	0.9972	NaCl <sub>5</sub>
0.9886	MgTi <sub>2</sub> S <sub>5</sub>	0.9975	NaBF <sub>4</sub>
0.9898	MgY <sub>2</sub> S <sub>4</sub>	0.9979	GaU
0.9898	MnTb <sub>2</sub> S <sub>4</sub>	0.9980	Fe <sub>2</sub> Ti <sub>5</sub>
0.9898	MnY <sub>2</sub> S <sub>4</sub>	0.9986	CaS <sub>4</sub>
0.9905	MgEr <sub>2</sub> S <sub>4</sub>	1.0000	CrYb <sub>2</sub> S <sub>4</sub>
0.9905	MgHo <sub>2</sub> S <sub>4</sub>	1.0000	CrTm <sub>2</sub> S <sub>4</sub>
0.9905	MnHo <sub>2</sub> S <sub>4</sub>	1.0000	CrEr <sub>2</sub> S <sub>4</sub>
0.9906	MgTb <sub>2</sub> S <sub>4</sub>	1.0000	CrHo <sub>2</sub> S <sub>4</sub>
0.9912	FeYb <sub>2</sub> S <sub>4</sub>	1.0000	CrY <sub>2</sub> S <sub>4</sub>
0.9913	MnEr <sub>2</sub> S <sub>4</sub>	1.0000	Co(NH <sub>3</sub> ) <sub>5</sub> N <sub>6</sub> Cl <sub>2</sub>

## Organic

0.1779	BMo <sub>2</sub> C	0.7540	ECr <sub>7</sub> C <sub>4</sub>
0.3929	C <sub>12</sub> H <sub>10</sub> S <sub>2</sub>	0.7729	(CH <sub>3</sub> N <sub>6</sub> ) <sub>2</sub>
0.4645	CH <sub>3</sub> NH <sub>3</sub> NiCl <sub>3</sub>	0.8327	(CH <sub>3</sub> ) <sub>3</sub> SnCN
0.5092	CBr <sub>4</sub> C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>	0.8482	ZnCS <sub>3</sub> (NH <sub>3</sub> ) <sub>2</sub>
0.5457	Ag <sup>+</sup> CN	0.8719	(CH <sub>3</sub> ) <sub>4</sub> N <sup>+</sup> HS <sup>-</sup> H <sub>2</sub> S
0.5985	KI·Hg(CN) <sub>2</sub>	0.8801	TiCl <sub>4</sub> ·C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>
0.6511	(C <sub>4</sub> H <sub>6</sub> Co(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> ) <sub>2</sub>	0.8881	CH <sub>3</sub> SH
0.7149	C <sub>6</sub> H <sub>6</sub> AgCl <sub>4</sub>	0.9160	(CH <sub>3</sub> ) <sub>2</sub> S <sub>2</sub>
0.7417	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> Na <sub>2</sub> S <sub>2</sub> ·2.5H <sub>2</sub> O	0.9731	SCNH(CH <sub>2</sub> ) <sub>6</sub> NH·C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>4</sub> ·SH
0.7516	Cr <sub>2</sub> VC <sub>2</sub>		

 $\begin{matrix} 2 & 2 & 2 \\ m & m & m \end{matrix}$ Cmca  $D_{2h}^{18}$  No. 64Inorganic - 32  
Organic - 11

## Inorganic

0.3345	Au <sub>3</sub> Zn	0.7418	I <sub>2</sub>
0.3391	Bi <sub>2</sub> S <sub>2</sub> Mo <sub>4</sub>	0.7423	I <sub>2</sub>
0.4129	As	0.7554	Cl <sub>2</sub>
0.4161	AsP	0.7649	Br <sub>2</sub>
0.4177	P	0.8048	Na <sub>2</sub> Mo <sub>2</sub> S <sub>7</sub>
0.4657	(NH <sub>4</sub> ) <sub>2</sub> CuCl <sub>4</sub>	0.8059	MoCl <sub>2</sub>
0.5669	(NH <sub>4</sub> ) <sub>2</sub> BeF <sub>4</sub>	0.8466	(NH <sub>4</sub> ) <sub>4</sub> P <sub>4</sub> S <sub>12</sub>
0.5725	Tl(As,Sb) <sub>3</sub> S <sub>5</sub>	0.8680	(NH <sub>4</sub> ) <sub>4</sub> P <sub>4</sub> S <sub>12</sub>
0.5728	Ce <sub>2</sub> (S <sub>4</sub> ) <sub>3</sub> ·8H <sub>2</sub> O	0.9221	Re <sub>2</sub> U
0.5906	Ga	0.9621	K <sub>2</sub> S <sub>2</sub>
0.6246	Na <sub>6</sub> P <sub>6</sub> S <sub>18</sub> ·6H <sub>2</sub> O	0.9637	T <sub>6</sub> I <sub>14</sub>
0.6495	Se(CN) <sub>2</sub>	0.9780	(W <sub>6</sub> Br <sub>6</sub> )(Br <sub>4</sub> ) <sub>2</sub>
0.7196	Zn <sub>3</sub> (V <sub>4</sub> ) <sub>2</sub>	0.9783	K <sub>4</sub> (HSi <sub>3</sub> ) <sub>4</sub>
0.7232	Co <sub>3</sub> (V <sub>4</sub> ) <sub>2</sub>	0.9820	Ba <sub>4</sub> PtI <sub>2</sub> S <sub>10</sub>
0.7239	Co <sub>3</sub> (V <sub>4</sub> ) <sub>2</sub>	0.9853	IF <sub>7</sub>
0.7243	AgN <sub>3</sub>	1.0000	(NH <sub>3</sub> ) <sub>2</sub> BH <sub>2</sub> Cl

## Organic

0.3563	CH <sub>3</sub> C <sup>+</sup> NH <sup>-</sup> NHC <sup>+</sup> CH <sub>3</sub>	0.6246	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> S
0.4100	CH <sub>3</sub> SH <sub>2</sub> ·HCl	0.6495	Se(CN) <sub>2</sub>
0.5151	C <sub>4</sub> H <sub>3</sub> SC <sup>+</sup> Ag	0.7805	AlH <sub>3</sub> ·2N(CH <sub>3</sub> ) <sub>3</sub>
0.5338	[(CH <sub>3</sub> ) <sub>2</sub> N] <sub>2</sub> S <sub>2</sub>	0.7900	N(C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> I <sub>7</sub>
0.5470	C <sub>2</sub> H <sub>2</sub> I <sub>2</sub>	0.9891	NaU <sub>2</sub> [S <sub>2</sub> CN(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ] <sub>3</sub> ·3H <sub>2</sub> O
0.5879	C <sub>2</sub> H <sub>4</sub> I <sub>2</sub>		

 $\begin{matrix} 2 & 2 & 2 \\ m & m & m \end{matrix}$ Cmmm  $D_{2h}^{19}$  No. 65Inorganic - 13  
Organic - 4

## Inorganic

0.0943	Ga <sub>13</sub> Nb <sub>5</sub>	0.2500	Ge <sub>2</sub> Th <sub>0.9</sub>
0.1900	Nb <sub>3</sub> S <sub>7</sub> F	0.4938	Cu <sub>2</sub> S
0.2340	As <sub>2</sub> CoFeS <sub>2</sub>	0.5873	Na <sub>2</sub> U <sub>4</sub>
0.2450	(Co,Fe)AsS	0.6665	(NH <sub>4</sub> ) <sub>2</sub> CuCl <sub>3</sub>

Cmmm  $D_{2h}^{19}$  No. 65 (continued)

## Inorganic (continued)

0.8473  $\text{NaCa}_3\text{UO}_2(\text{CO}_3)_3\text{SO}_4\text{Fe}10\text{H}_2\text{O}$   
 0.8580  $\text{Mg}_8\text{Fe}_4\text{Al}_{26}\text{B}_3\text{Si}_{15}\text{O}_{86}$   
 0.8593  $\text{Fe}_3\text{Mg}_{11}\text{Al}_{25}\text{B}_3\text{Si}_{15}\text{O}_{86}$

0.9027  $\text{NaIO}_3$   
 0.9264  $\text{Ga}_3\text{Pt}_5$

## Organic

0.5061  $(\text{C}_5\text{H}_5\text{NH})\text{HReCl}_4$   
 0.5108  $\text{C}_{16}\text{H}_{12}\text{N}_2\text{O}_3$

0.7078  $\text{Cd}[\text{OC}(\text{NH}_2)_2]_2\text{Cl}_2$   
 0.8473  $\text{NaCa}_3\text{UO}_2(\text{CO}_3)_3\text{SO}_4\text{Fe}10\text{H}_2\text{O}$

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$

Cccm  $D_{2h}^{20}$  No. 66

Inorganic - 4  
 Organic - 0

## Inorganic

0.5678  $\text{Al}_3\text{Mg}_2(\text{Si}_5\text{Al})\text{O}_{18}$   
 0.5700  $(\text{Mg}, \text{Fe}, \text{Mn})_2\text{Al}_4\text{Si}_5\text{O}_{18} \cdot n\text{H}_2\text{O}$

0.7203  $\text{Ca}_3\text{Nb}_2\text{O}_8$   
 0.7409  $\text{Fe}_2\text{Pb}(\text{OH})_2(\text{AsO}_4)_2$

## Organic

.....

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$

Cmma  $D_{2h}^{21}$  No. 67

Inorganic - 9  
 Organic - 3

## Inorganic

0.3843  $(\text{Mn}, \text{Ca})_{25}(\text{Zn}, \text{Mg}, \text{Fe})_{15}(\text{AsO}_4)_7(\text{OH})_{33}\text{O}_{13}$   
 0.4664  $\text{NiU}_3\text{O}_{10}$   
 0.4669  $\text{FeU}_3\text{O}_{10}$   
 0.4721  $\text{UTiO}_5$   
 0.4912  $\text{Ag}_3\text{Pb}_2\text{Sb}_3\text{S}_8$

0.5996  $\text{RbHSO}_4$   
 0.6600  $\text{NH}_4\text{H}_2\text{PO}_2$   
 0.6935  $\text{E}_{10}\text{H}_{14}$   
 0.7871  $\text{Al}_8\text{Ca}_3(\text{OH})_6(\text{PO}_4)_8 \cdot 15\text{H}_2\text{O}$

## Organic

0.2859  $\text{C}_{23}\text{H}_{45}\text{O}_2\text{KOC}_{23}\text{H}_{46}\text{O}_2$   
 0.4206  $\text{N}_6\text{O}_2\text{C}_6\text{H}_4\text{N}:\text{NPF}_6$

0.6309  $\text{C}_{22}\text{H}_{16}$

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$

Ccca  $D_{2h}^{22}$  No. 68

Inorganic - 3  
 Organic - 5

## Inorganic

0.6812  $\text{MnAl}_2\text{Si}_2\text{O}_6(\text{OH})_4$   
 0.6823  $\text{Al}_2\text{Fe}(\text{OH})_4(\text{SiO}_3)_2$

0.6885  $\text{Al}_2\text{Mn}[(\text{OH})_4(\text{SiO}_3)_2]$

## Organic

0.6655  $\text{C}_9\text{H}_6\text{NCHCl}_2$   
 0.6789  $\text{C}_{18}\text{H}_{24}$   
 0.8837  $\text{Pd}(\text{C}_5\text{H}_8\text{NO})_2$

0.8994  $\text{Cu}(\text{C}_5\text{H}_8\text{NO})_2$   
 0.9042  $\text{Ni}(\text{C}_5\text{H}_8\text{NO})_2$

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$

Fmmm  $D_{2h}^{23}$  No. 69

Inorganic - 22  
 Organic - 4

## Inorganic

0.1659  $\text{Bi}_4\text{Tl}_3\text{O}_{12}$   
 0.1818  $\text{C}$   
 0.2030  $\text{NaBi}_5\text{Nb}_4\text{O}_{18}$   
 0.2155  $\text{PbBi}_2\text{Nb}_2\text{O}_9$   
 0.2161  $\text{Bi}_3\text{TaTiO}_9$   
 0.2165  $\text{BaBi}_2\text{Nb}_2\text{O}_9$   
 0.2167  $\text{Bi}_3\text{NbTiO}_9$   
 0.2180  $\text{KBi}_5\text{Nb}_4\text{O}_{18}$   
 0.2197  $\text{SrBi}_2\text{Nb}_2\text{O}_9$   
 0.2198  $\text{SrBi}_2\text{Ta}_2\text{O}_9$   
 0.2205  $\text{CaBi}_2\text{Nb}_2\text{O}_9$

0.2401  $\text{Pb}_7\text{O}_6\text{Br}_2$   
 0.2402  $\text{Pb}_7\text{O}_6\text{Cl}_2$   
 0.3259  $\text{Al}_3\text{Fe}$   
 0.3974  $\text{Bi}_2\text{O}_2(\text{CO}_3)$   
 0.5111  $\text{Na}_2\text{UO}_4$   
 0.5746  $\text{Pb}_7\text{O}_6\text{Br}_2$   
 0.5760  $\text{Li}_2\text{UO}_4$   
 0.6340  $\text{UO}_2(\text{OH})_2$   
 0.7064  $\text{Ca}_2\text{CuK}_2(\text{SO}_4)_4 \cdot 2\text{H}_2\text{O}$   
 0.9038  $\text{TLF}$   
 0.9934  $\text{Pa}$

Fmmm  $D_{2h}^{23}$  No. 69 (continued)

Organic			
0.1818	C	0.9660	$[(C_2H_5)_4N]_2UCl_6$
0.5666	$C_6(CH_3)_6$	0.9793	$[(C_2H_5)_4N]_2PuCl_6$

 $\frac{2}{m} \frac{2}{m} \frac{2}{m}$ Fddd  $D_{2h}^{24}$  No. 70Inorganic - 49  
Organic - 5

Inorganic			
0.4159	$Ge_{1.6}Th$	0.5255	$S_8$
0.4450	$Zr(SO_4)_2 \cdot 4H_2O$	0.5304	$Al_2(PO_4)_2F_2(OH) \cdot 7H_2O$
0.4483	$Zr(SO_4)_2 \cdot 4H_2O$	0.5600	$Si_2Ti$
0.4696	$Er_2Se_3$	0.5682	$Pu$
0.4699	$Y_2Se_3$	0.5991	$(UO_2)_5(OH)_2(SiO_4)_2 \cdot 5H_2O$
0.4701	$Lu_2Se_3$	0.7413	$UV_3O_{10}$
0.4701	$Yb_2Se_3$	0.7933	$Na_2SO_4$
0.4702	$Ho_2Se_3$	0.7970	$Ag_2SeO_4$
0.4703	$Tm_2Se_3$	0.7982	$Na_2SO_4$
0.4712	$IrCl_3$	0.8063	$Ba(MnO_4)_2$
0.4715	$Lu_2Te_3$	0.8072	$Na_2SeO_4$
0.4715	$Tm_2Te_3$	0.8103	$Ag_2SO_4$
0.4715	$Er_2Te_3$	0.8228	$Cd_2SiO_4$
0.4715	$Tb_2Te_3$	0.8563	$NaNH_2$
0.4716	$Ho_2Te_3$	0.9120	$Al_2Ru$
0.4716	$Y_2Te_3$	0.9129	$Al_2Ru$
0.4716	$Dy_2Te_3$	0.9271	$Al_{1.3}MnSi_{0.7}$
0.4721	$Sc_2(Se,Te)_3$	0.9407	$(Al_{1.3}Si_{0.7})Mo$
0.4722	$Sc_2Se_3$	0.9411	$Ga_2Ru$
0.4970	$CuMg_2$	0.9426	$Pt(NH_3)_2Br_2 \cdot Pt(NH_3)_2Br_4$
0.5019	$EMn_4$	0.9557	$(Ga_{0.7}Ge_{0.3})_2Mo$
0.5019	$BCr_4$	0.9647	$Sn_2Zr$
0.5086	$Sn_3V_2$	0.9663	$Si_2Ti$
0.5148	$Nb_2Sn_3$	0.9704	$Sr(N_3)_2$
0.5155	$NbSn_2$		

Organic			
0.4605	$C_6H_{12}Br_2N_4S_2Te$	0.9834	$KS_2P(OCH_3)_2$
0.6536	$Cl_5C_5H_4N_4$	0.9988	$C_{13}H_{10}N_2 \cdot 0.5H_2O$
0.9356	$C_{11}H_9N_2O_3Br$		

 $\frac{2}{m} \frac{2}{m} \frac{2}{m}$ Inmmm  $D_{2h}^{25}$  No. 71Inorganic - 40  
Organic - 4

Inorganic			
0.1897	$C_3Si_2U_3$	0.6102	$Ag_2Te$
0.2358	$B_4Mn_3$	0.6434	$Pb_2(Cu,Fe)_{21}S_{15}$
0.2374	$B_4Ti_3$	0.6439	$B_2CoMo_2$
0.4467	$Pd_2Ta$	0.6441	$B_2Mo_2Ni$
0.4514	$Pd_2Ta$	0.6442	$B_2NiW_2$
0.4532	$Pd_2V$	0.6446	$B_2CoW_2$
0.4539	$Pt_2V$	0.6471	$B_2FeW_2$
0.4591	$Ni_2V$	0.7302	$Al_9(Li,Na)_4Sr(OH)_9(PO_4)_8$
0.4645	$Ni_2V$	0.7326	$PdPt(NH_3)_4Cl_6$
0.4671	$NbPt_2$	0.7338	$(SbO)_8(OH)_6Cl_2 \cdot H_2O$
0.4680	$NbPt_2$	0.7395	$(Na,K)_4Mg_2(Si_{30}Al_6)O_{72}(OH)_2 \cdot 18H_2O$
0.4747	$Na_2UF_6$	0.7403	$UO_4 \cdot 2H_2O$
0.5462	$Nb_6Sn_5$	0.7410	$Pt_2(NH_3)_4Br_6$
0.5680	$Na_2MoF_6$	0.7514	$Pd_2(NH_3)_4Cl_6$
0.5720	$Na_2OsF_6$	0.8396	$NaCN$
0.5743	$Na_2SnF_6$	0.8457	$Rb_2O_2$
0.5752	$Na_2ReF_6$	0.8554	$Cs_2O_2$
0.5792	$Na_2PbF_6$	0.8878	$C_2Li_2$
0.6011	$CsFeS_2$	0.9384	$NaN_3$
0.6040	$CsFeSe_2$	0.9630	$PdCl_3 \cdot 2NH_3$

Organic			
0.1897	$Si_2U_3C_3$	0.8396	$NaCN$
0.3687	$NaCl \cdot C_6(NH_2)_2 \cdot H_2O$	0.8878	$Li_2C_2$

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	Ibam	$D_{2h}^{26}$	No. 72	Inorganic - 15	Organic - 10
Inorganic					
0.3278	Au <sub>5</sub> Zn <sub>3</sub>		0.6172	Si $\theta$ <sub>2</sub>	
0.5119	Ga <sub>2</sub> Mg <sub>5</sub>		0.6178	SiSe <sub>2</sub>	
0.5172	In <sub>2</sub> Mg <sub>5</sub>		0.7029	H <sub>2</sub> $\theta$	
0.5368	BeBr <sub>2</sub>		0.7385	Au <sub>5</sub> GaZn <sub>2</sub>	
0.5403	BeI <sub>2</sub>		0.9787	Hg <sub>5</sub> $\theta$ <sub>4</sub> Cl <sub>2</sub>	
0.5436	BeCl <sub>2</sub>		0.9818	AgN <sub>3</sub>	
0.5694	K <sub>2</sub> Zn $\theta$ <sub>2</sub>		0.9880	Hg( $\theta$ Hg) <sub>4</sub> Br <sub>2</sub>	
0.5864	SiS <sub>2</sub>				
Organic					
0.3743	Cu(C <sub>8</sub> H <sub>8</sub> N $\theta$ ) <sub>2</sub>		0.6259	Ni(C <sub>4</sub> H <sub>7</sub> N <sub>2</sub> $\theta$ <sub>2</sub> ) <sub>2</sub>	
0.5209	[(CH <sub>3</sub> ) <sub>2</sub> Mg] <sub>n</sub>		0.6330	(C <sub>4</sub> H <sub>7</sub> N <sub>2</sub> $\theta$ <sub>2</sub> ) <sub>2</sub> Pt	
0.5317	(CH <sub>3</sub> ) <sub>2</sub> Be		0.8486	CH <sub>2</sub> =CH-C $\theta$ $\theta$ H	
0.5566	(C <sub>5</sub> H <sub>14</sub> N $\theta$ )[Cr(NCS) <sub>4</sub> (NH <sub>3</sub> ) <sub>2</sub> ]		0.8662	CH <sub>2</sub> :CH-C $\theta$ $\theta$ H	
0.6225	Pd(C <sub>4</sub> H <sub>7</sub> N <sub>2</sub> $\theta$ <sub>2</sub> ) <sub>2</sub>		0.9977	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> $\theta$ <sub>2</sub>	

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	Ibca	$D_{2h}^{27}$	No. 73	Inorganic - 4	Organic - 3
Inorganic					
0.2941	AgKCl <sub>3</sub>		0.9890	AlAs <sub>2</sub> Li <sub>3</sub>	
0.6894	Na <sub>2</sub> Si $\theta$ <sub>3</sub> •9H <sub>2</sub> $\theta$		0.9897	AlLi <sub>3</sub> P <sub>2</sub>	
Organic					
0.2941	AgKCl <sub>3</sub>		0.7555	C <sub>8</sub> H <sub>4</sub> KN <sub>5</sub> $\theta$ <sub>6</sub> •2H <sub>2</sub> $\theta$	
0.6869	C <sub>6</sub> H <sub>2</sub> (N $\theta$ <sub>2</sub> ) <sub>3</sub> $\theta$ NH <sub>4</sub>				

$\frac{2}{m} \frac{2}{m} \frac{2}{m}$	Imma	$D_{2h}^{28}$	No. 74	Inorganic - 48	Organic - 2
Inorganic					
0.3028	DySi <sub>2</sub>		0.9258	Cu <sub>2</sub> Er	
0.3031	Si <sub>2</sub> Y		0.9272	Cu <sub>2</sub> Ho	
0.3043	GdSi <sub>2</sub>		0.9304	Cu <sub>2</sub> Dy	
0.3050	Si <sub>2</sub> Sm		0.9316	CeCu <sub>2</sub>	
0.3083	NdSi <sub>2</sub>		0.9324	Cu <sub>2</sub> Tb	
0.3092	PrSi <sub>2</sub>		0.9334	Ag <sub>2</sub> Sr	
0.3099	CeGe <sub>2</sub>		0.9346	CoU $\theta$ <sub>4</sub>	
0.3108	Ge <sub>2</sub> La		0.9356	Cu <sub>2</sub> Gd	
0.3744	Hg <sub>2</sub> (Cl $\theta$ <sub>4</sub> ) <sub>2</sub> •4H <sub>2</sub> $\theta$		0.9373	Cd <sub>2</sub> Eu	
0.3813	Ca <sub>2</sub> (Fe,Al) <sub>2</sub> $\theta$ <sub>5</sub>		0.9390	Cu <sub>2</sub> Sm	
0.3816	Ca <sub>2</sub> Fe <sub>2</sub> $\theta$ <sub>5</sub>		0.9415	NiU $\theta$ <sub>4</sub>	
0.4573	Al <sub>4</sub> U		0.9436	Cu <sub>2</sub> Y	
0.4583	Al <sub>4</sub> Pu		0.9447	Cu <sub>2</sub> Pr	
0.4713	LiGaTi $\theta$ <sub>4</sub>		0.9479	Cd <sub>2</sub> Sr	
0.6103	Ni(CN) <sub>2</sub> NH <sub>3</sub> •nH <sub>2</sub> $\theta$		0.9506	Zn(NH <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	
0.6498	Al <sub>4</sub> Na <sub>4</sub> ( $\theta$ H) <sub>8</sub> (C $\theta$ <sub>3</sub> ) <sub>4</sub>		0.9513	Cu <sub>2</sub> Nd	
0.6640	CuLiV $\theta$ <sub>4</sub>		0.9525	MgU $\theta$ <sub>4</sub>	
0.7088	Fe <sub>3</sub> $\theta$ <sub>4</sub>		0.9538	Ag <sub>2</sub> Ba	
0.7516	NaPF <sub>6</sub> •H <sub>2</sub> $\theta$		0.9546	Zn(NH <sub>3</sub> ) <sub>2</sub> Br <sub>2</sub>	
0.9135	Cu <sub>2</sub> Yb		0.9570	CaZn <sub>2</sub>	
0.9179	Ag <sub>2</sub> Eu		0.9615	Cu <sub>2</sub> Eu	
0.9179	Cu <sub>2</sub> Lu		0.9665	MnU $\theta$ <sub>4</sub>	
0.9236	Hg <sub>2</sub> K		0.9770	AlB <sub>12</sub>	
0.9241	Cu <sub>2</sub> Tm		0.9993	EuZn <sub>2</sub>	
Organic					
0.6103	Ni(CN) <sub>2</sub> NH <sub>3</sub> •nH <sub>2</sub> $\theta$		0.6498	Al <sub>4</sub> Na <sub>4</sub> ( $\theta$ H) <sub>8</sub> (C $\theta$ <sub>3</sub> ) <sub>4</sub>	

4	P4	$C_4^1$	No. 75	Inorganic - 1 Organic - 0
Inorganic				
1.0207	Pt(NH <sub>3</sub> ) <sub>4</sub> PtCl <sub>4</sub>			
Organic				
.....				
4	P4 <sub>1</sub>	$C_4^2$	No. 76 (includes P4 <sub>3</sub> No. 78)	Inorganic - 4 Organic - 12
Inorganic				
3.0000	Fe <sub>2</sub> O <sub>3</sub>			3.5824
3.4670	ISbCl <sub>8</sub>			3.6122
Organic				
0.7174	AgNi(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>3</sub> •2AgNO <sub>3</sub> •H <sub>2</sub> O			3.5703
0.7452	C <sub>33</sub> H <sub>38</sub> O <sub>7</sub>			3.997
0.8678	C <sub>22</sub> H <sub>29</sub> ClO <sub>7</sub>			4.028
2.2462	C <sub>5</sub> H <sub>10</sub> (CN) <sub>2</sub>			5.3464
2.364	C <sub>28</sub> H <sub>36</sub> N <sub>4</sub>			5.449
2.472	(CH <sub>2</sub> CO) <sub>2</sub> NI			5.4600
				C <sub>36</sub> H <sub>45</sub> N <sub>17</sub> •C <sub>3</sub> H <sub>6</sub> O
				C <sub>15</sub> H <sub>15</sub> O <sub>6</sub> Br
				C <sub>15</sub> H <sub>15</sub> O <sub>6</sub> Cl
				C <sub>14</sub> H <sub>8</sub> O <sub>4</sub>
				C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> •HBr
				C <sub>14</sub> H <sub>8</sub> O <sub>4</sub>
4	P4 <sub>2</sub>	$C_4^3$	No. 77	Inorganic - 3 Organic - 0
Inorganic				
0.6133	H <sub>2</sub> S			1.2256
1.0752	MgB <sub>2</sub> O(OH) <sub>6</sub>			NH <sub>4</sub> NO <sub>3</sub>
Organic				
.....				
4	P4 <sub>3</sub>	$C_4^4$	No. 78 (see No. 76)	
.....				
4	I4	$C_4^5$	No. 79	Inorganic - 6 Organic - 5
Inorganic				
0.4386	WOFr <sub>4</sub>			1.3828
0.4711	WCl <sub>4</sub>			1.7284
0.8178	H <sub>2</sub>			1.7303
Organic				
0.2867	CH <sub>3</sub> •CH(NH <sub>2</sub> )•CO•NH•CH(CH <sub>3</sub> )•COOH			1.5503
0.395	(CH <sub>3</sub> CHO) <sub>4</sub>			1.6397
0.7256	C <sub>44</sub> H <sub>29</sub> FeN <sub>4</sub> O•H <sub>2</sub> O			
				[Rh(CH <sub>3</sub> COO) <sub>2</sub> Br] <sub>2</sub> •2(NH)C(NH <sub>2</sub> ) <sub>2</sub>
				[Rh(CH <sub>2</sub> COO) <sub>2</sub> Cl] <sub>2</sub> •2(NH)C(NH <sub>2</sub> ) <sub>2</sub>
4	I4 <sub>1</sub>	$C_4^6$	No. 80	Inorganic - 0 Organic - 3
Inorganic				
.....				

I<sub>4</sub> C<sub>4</sub><sup>6</sup> No. 80 (continued)

## Organic

0.8596 (C<sub>6</sub>H<sub>5</sub>)<sub>2</sub>TeBr<sub>2</sub> 2.4677 C<sub>6</sub>H<sub>7</sub>N<sup>6</sup>  
 2.4336 PdI(C<sub>6</sub>H<sub>4</sub>[As(CH<sub>3</sub>)<sub>2</sub>]<sub>2</sub>)<sub>2</sub>•Cl<sub>4</sub>

4

P<sub>4</sub> S<sub>4</sub><sup>1</sup> No. 81Inorganic - 2  
Organic - 9

## Inorganic

0.6583 (Ca,Na)<sub>2</sub>Be(Si,Al)<sub>2</sub>(O,F)<sub>7</sub> 7.2826 Au(Pb,Sb,Fe)<sub>8</sub>(S,Te)<sub>11</sub>

## Organic

0.3751 (H<sup>6</sup>•C<sub>6</sub>H<sub>4</sub>•CH:N•C<sub>4</sub>H<sub>9</sub>)<sub>2</sub>Zn 0.5242 (C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>NHC<sub>3</sub>•32.0H<sub>2</sub>O  
 0.5209 [(C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>N]<sub>2</sub>C<sub>2</sub>•64H<sub>2</sub>O 0.5259 [(C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>N]<sub>2</sub>W<sub>4</sub>•62.7H<sub>2</sub>O  
 0.5236 [(C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>N]<sub>2</sub>Cr<sub>4</sub>•65.1H<sub>2</sub>O 0.5285 (C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>NBr•32.6H<sub>2</sub>O  
 0.5240 [(C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>N]<sub>2</sub>HP<sub>4</sub>•64.2H<sub>2</sub>O 0.5305 (C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>NCl•33.8H<sub>2</sub>O  
 0.5241 (C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>N<sup>6</sup>•CCH<sub>3</sub>•31.3H<sub>2</sub>O

4

I<sub>4</sub> S<sub>4</sub><sup>2</sup> No. 82Inorganic - 54  
Organic - 27

## Inorganic

0.1453 W<sub>3</sub>Nb<sub>18</sub>O<sub>69</sub> 1.8548 CdAl<sub>2</sub>S<sub>4</sub>  
 0.1819 W<sub>3</sub>Nb<sub>14</sub>O<sub>44</sub> 1.8576 HgGa<sub>2</sub>S<sub>4</sub>  
 0.2454 Nb<sub>18</sub>P<sub>2</sub>O<sub>50</sub> 1.8584 CdAl<sub>2</sub>Se<sub>4</sub>  
 0.3675 CdHg(CNS)<sub>4</sub> 1.8684 CdGa<sub>2</sub>Se<sub>4</sub>  
 0.3746 NH<sub>4</sub>Cu<sub>7</sub>S<sub>4</sub> 1.8695 HgAl<sub>2</sub>S<sub>4</sub>  
 0.3935 CoHg(CNS)<sub>4</sub> 1.8777 Li<sub>2</sub>Mg<sub>2</sub>(NH)<sub>3</sub>  
 0.4004 ZnHg(CNS)<sub>4</sub> 1.8816 HgAl<sub>2</sub>Se<sub>4</sub>  
 0.4149 CoHg(SeCN)<sub>4</sub> 1.8866 HgGa<sub>2</sub>Se<sub>4</sub>  
 0.4834 AsPd<sub>3</sub> 1.9383 CdGa<sub>2</sub>Te<sub>4</sub>  
 0.4897 Fe<sub>3</sub>P 1.9795 ZnGa<sub>2</sub>S<sub>4</sub>  
 0.4902 Ni<sub>3</sub>P 1.9815 ZnAl<sub>2</sub>Se<sub>4</sub>  
 0.4903 Fe<sub>3</sub>P 1.9821 Hg<sub>2</sub>GeSe<sub>4</sub>  
 0.4909 (Fe,Ni,Co)<sub>3</sub>P 1.9993 ZnGa<sub>2</sub>Te<sub>4</sub>  
 0.4975 Mn<sub>3</sub>P 1.9993 HgGa<sub>2</sub>Te<sub>4</sub>  
 0.4995 Cr<sub>3</sub>P 1.9996 ZnGa<sub>2</sub>Se<sub>4</sub>  
 0.5510 KAg<sup>6</sup> 1.9996 ZnIn<sub>2</sub>Se<sub>4</sub>  
 0.6092 SbCl<sub>4</sub>F 2.0000 AgIn<sub>5</sub>Se<sub>8</sub>  
 0.6168 TaCl<sub>4</sub>F 2.0000 CdIn<sub>2</sub>Te<sub>4</sub>  
 0.8608 Ca<sub>4</sub>B<sub>2</sub>As<sub>2</sub>O<sub>12</sub>•4H<sub>2</sub>O 2.0000 Ag<sub>2</sub>HgI<sub>4</sub>  
 0.8724 Ca<sub>2</sub>B(OH)<sub>4</sub>As<sub>2</sub>O<sub>4</sub> 2.0002 ZnIn<sub>2</sub>Te<sub>4</sub>  
 1.0273 Na<sub>8</sub>Al<sub>2</sub>Be<sub>2</sub>Si<sub>8</sub>O<sub>24</sub>(Cl,S)<sub>2</sub> 2.0010 HgIn<sub>2</sub>Te<sub>4</sub>  
 1.3551 AlAs<sub>4</sub> 2.0170 HgAl<sub>2</sub>Te<sub>4</sub>  
 1.3608 AlP<sub>4</sub> 2.0313 CdAl<sub>2</sub>Te<sub>4</sub>  
 1.5245 BaS<sub>4</sub> 2.0355 ZnAl<sub>2</sub>Te<sub>4</sub>  
 1.5328 BP<sub>4</sub> 2.0375 LiNH<sub>2</sub>  
 1.5367 BeS<sub>4</sub> 2.0472 HgIn<sub>2</sub>Se<sub>4</sub>  
 1.8074 CdGa<sub>2</sub>S<sub>4</sub> 2.2218 LiHS

## Organic

0.2472 Hg(CH<sub>4</sub>N<sub>2</sub>S)<sub>4</sub>Co(SCN)<sub>4</sub> 0.5810 (C<sub>6</sub>H<sub>5</sub>)<sub>4</sub>AsI  
 0.2826 C<sub>20</sub>H<sub>24</sub>NNa<sub>3</sub>O<sub>16</sub>S<sub>4</sub> 0.586 (C<sub>6</sub>H<sub>5</sub>)<sub>4</sub>PI  
 0.3142 C<sub>48</sub>H<sub>36</sub>Si 0.6608 (PN[N(CH<sub>3</sub>)<sub>2</sub>]<sub>2</sub>)<sub>4</sub>  
 0.3675 CdHg(CNS)<sub>4</sub> 0.6843 C(CH<sub>2</sub>•C<sub>6</sub>H<sub>5</sub>)<sub>4</sub>  
 0.3855 C<sub>17</sub>H<sub>20</sub>N<sub>2</sub>SeHBr 0.6890 Cu(C<sub>2</sub>H<sub>5</sub>N)<sub>4</sub>(NO<sub>3</sub>)<sub>2</sub>  
 0.3935 CoHg(CNS)<sub>4</sub> 0.7835 N(C<sub>2</sub>H<sub>5</sub>)<sub>4</sub>I  
 0.4004 ZnHg(CNS)<sub>4</sub> 0.9222 Fe[SC(NH<sub>2</sub>)<sub>2</sub>]<sub>4</sub>Cl<sub>2</sub>  
 0.4149 CoHg(SeCN)<sub>4</sub> 0.9267 Mn[SC(NH<sub>2</sub>)<sub>2</sub>]<sub>4</sub>Cl<sub>2</sub>  
 0.4265 Ag(SC<sub>2</sub>H<sub>5</sub>N)<sub>4</sub>Cl 0.9397 Ni[SC(NH<sub>2</sub>)<sub>2</sub>]<sub>4</sub>Cl<sub>2</sub>  
 0.4393 Cu(S:CCH<sub>3</sub>•NH<sub>2</sub>)<sub>4</sub>Cl 0.9458 Co[SC(NH<sub>2</sub>)<sub>2</sub>]<sub>4</sub>Cl<sub>2</sub>  
 0.455 Sn(C<sub>6</sub>H<sub>4</sub>•CH<sub>3</sub>)<sub>4</sub> 0.9564 Cd[SC(NH<sub>2</sub>)<sub>2</sub>]<sub>4</sub>Cl<sub>2</sub>  
 0.471 Sn(C<sub>6</sub>H<sub>4</sub>CH<sub>3</sub>)<sub>4</sub> 1.3252 (C<sub>3</sub>H<sub>7</sub>)<sub>4</sub>NBr  
 0.5352 C<sub>4</sub>H<sub>6</sub>F<sub>2</sub>O<sub>2</sub> 1.4345 C(CH<sub>2</sub>•H)<sub>4</sub>  
 0.5433 (C<sub>6</sub>H<sub>5</sub>)<sub>4</sub>AsFeCl<sub>4</sub>

$\frac{4}{m}$	P4/m	$C_{4h}^1$	No. 83	Inorganic - 1 Organic - 1
Inorganic				
0.6230	$Na_4ClSi_9Al_3O_{24}$			
Organic				
1.1429	$Ni(CN)_2NH_3 \cdot C_6H_6$			
$\frac{4}{m}$	P4 <sub>2</sub> /m	$C_{4h}^2$	No. 84	Inorganic - 3 Organic - 3
Inorganic				
0.6270	$3NaAlSi_3O_8 \cdot NaCl$		1.0330	(Pt, Pd, Ni)S
1.0311	PdS			
Organic				
0.5229	$(C_4H_9)_4NF \cdot 32.8H_2O$		0.770	$C(C_6H_5)_4$
0.7318	$Mg(C_2H_5)_2$			
$\frac{4}{m}$	P4/n	$C_{4h}^3$	No. 85	Inorganic - 18 Organic - 2
Inorganic				
0.4557	$K_2NaClS_2O_6$		0.9038	$CuBO_2Cl \cdot 2H_2O$
0.4941	$FeF_3 \cdot 3H_2O$		0.9063	$CuBO_2Cl \cdot 2H_2O$
0.5011	$KMg(Cl, Br)_3 \cdot 6H_2O$		1.0668	$NH_4CuSiF_7 \cdot 4H_2O$
0.5241	$InF_3 \cdot 3H_2O$		1.0782	$NH_4CuTiF_7 \cdot 4H_2O$
0.6425	$NbOP_4$		1.0877	$NH_4CuSnF_7 \cdot 4H_2O$
0.6454	$VO_4$		1.0924	$NH_4CuWO_2F_5 \cdot 4H_2O$
0.7327	$NH_4I \cdot 4NH_3$		1.2079	$Mg(UO_2)_2(AsO_4)_2 \cdot 4H_2O$
0.8069	$PCl_5$		1.4883	$Tl_2Se$
0.8938	$Zr(I_3)_4$		2.4833	$Cu(UO_2)_2(P_4)_2 \cdot 8H_2O$
Organic				
0.3925	$[(C_2H_5)_2NCS_2]_2Ni$		0.6595	$Co[(C_6H_5)_2CH_3AsO_4]_4(ClO_4)_2$
$\frac{4}{m}$	P4 <sub>2</sub> /n	$C_{4h}^4$	No. 86	Inorganic - 35 Organic - 9
Inorganic				
0.2879	$Na_2Co(CNS)_4 \cdot 8H_2O$		1.0789	ZrD
0.3903	$(PNCl_2)_4$		1.9496	$Cd(NH_2SO_3)_2$
0.4863	$Hf_3P$		2.4943	$Cu(UO_2)_2(P_4)_2 \cdot 8H_2O$
0.4936	$PTa_3$		2.8214	$Mg(UO_2)_2(AsO_4)_2 \cdot 9H_2O$
0.4958	$PZr_3$		3.1454	AuI
0.4961	$AsTa_3$		5.9000	$LaTe_3$
0.4965	$Fe_3(P_{0.37}B_{0.63})$		5.9095	$CeTe_3$
0.4966	$AsZr_3$		5.9120	$NdTe_3$
0.4995	$PTa_3$		5.9131	$GdTe_3$
0.5027	$Nb_3P$		5.9164	$PrTe_3$
0.5045	$AsNb_3$		5.9170	$SmTe_3$
0.5067	$PV_3$		5.9207	$HoTe_3$
0.5374	$Ce(I_3)_4$		5.9211	$TbTe_3$
0.5497	$P_4N_4Cl_8$		5.9225	$ErTe_3$
0.5626	$(PNBr_2)_4$		5.9238	$YTe_3$
0.9741	$AgSb(OH)_6$		5.9241	$DyTe_3$
0.9838	$NaSb(OH)_6$		5.9289	$TmTe_3$
0.9894	$FeGe(OH)_6$			
Organic				
0.2879	$Na_2Co(CNS)_4 \cdot 8H_2O$		0.4869	$C_{13}H_{12}N_2O_2$
0.3672	$(C_6H_{11}P)_4$		0.5484	$Hg(CH_2C_6H_5)_2$
0.4019	$[(CH_3)_2SiO]_4$		0.692	$C_5H_{16}N_4 \cdot 4HCl$
0.459	$C(CH_2OC_6H_3)_4$		2.614	$CH_3 \cdot CH=N \cdot NH \cdot C_6H_3(N_2)_2$
0.4864	$In(CH_3)_3$			

$\frac{4}{m}$	I4/m $C_{4h}^5$	No. 87	Inorganic - 68 Organic - 11
Inorganic			
0.2000	Nb <sub>2</sub> S	0.3711	Ti <sub>5</sub> Te <sub>4</sub>
0.2871	(Ba, K)(Mn, Mn, Fe, Al) <sub>8</sub> (OH) <sub>16</sub>	0.4171	Na <sub>4n</sub> [Cu(NH <sub>3</sub> ) <sub>4</sub> ] <sub>n</sub> [Cu <sub>n</sub> (S <sub>2</sub> S <sub>3</sub> ) <sub>2n</sub> ] <sub>2</sub>
0.2885	Fe <sub>2</sub> OH	0.5864	Ni <sub>12</sub> P <sub>5</sub>
0.2901	Mn <sub>2</sub> O <sub>2</sub>	0.5944	CaC <sub>2</sub> O <sub>4</sub> •2H <sub>2</sub> O
0.2904	(K, Na)(Mn, Al, Si) <sub>8</sub> (OH) <sub>16</sub>	0.6117	Na <sub>4</sub> Np <sub>5</sub>
0.2904	Rb <sub>2</sub> (Ti <sub>2</sub> Ti <sub>6</sub> ) <sub>16</sub>	0.6126	Na <sub>4</sub> U <sub>5</sub>
0.2908	Rb <sub>2</sub> (Cr <sub>2</sub> Ti <sub>6</sub> ) <sub>16</sub>	0.6162	Na <sub>4</sub> Pu <sub>5</sub>
0.2909	K <sub>2</sub> (Ti <sub>2</sub> Ti <sub>6</sub> ) <sub>16</sub>	0.6201	Ni <sub>4</sub> W
0.2911	Rb <sub>2</sub> (Al <sub>2</sub> Ti <sub>6</sub> ) <sub>16</sub>	0.6201	Ca <sub>4</sub> Ce <sub>3</sub> Si <sub>6</sub> Al <sub>6</sub> O <sub>24</sub>
0.2911	Rb <sub>2</sub> (NiTi <sub>7</sub> ) <sub>16</sub>	0.6216	(Ca, Na, K) <sub>4</sub> ((Si, Al)(OH) <sub>2</sub> ) <sub>12</sub> (C <sub>2</sub> O <sub>3</sub> , HC <sub>2</sub> O <sub>3</sub> )
0.2915	Rb <sub>2</sub> (Ga <sub>2</sub> Ti <sub>6</sub> ) <sub>16</sub>	0.6220	Ca <sub>8</sub> (C <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> (Al <sub>2</sub> Si <sub>2</sub> O <sub>8</sub> ) <sub>6</sub>
0.2917	Rb <sub>2</sub> (ZnTi <sub>7</sub> ) <sub>16</sub>	0.6248	Au <sub>4</sub> Mn
0.2918	Rb <sub>2</sub> (MgTi <sub>7</sub> ) <sub>16</sub>	0.6255	3CaAl <sub>2</sub> Si <sub>2</sub> O <sub>8</sub> •CaC <sub>2</sub> O <sub>4</sub>
0.2919	K <sub>1.60</sub> (Al <sub>1.60</sub> Ti <sub>6.40</sub> ) <sub>16</sub>	0.6270	Na <sub>4</sub> Cl(AlSi <sub>3</sub> O <sub>8</sub> ) <sub>3</sub>
0.2919	K <sub>2</sub> (Cr <sub>2</sub> Ti <sub>6</sub> ) <sub>16</sub>	0.6605	KSb <sub>4</sub> F <sub>13</sub>
0.2919	Rb <sub>2</sub> (CoTi <sub>7</sub> ) <sub>16</sub>	0.6616	Li <sub>4</sub> Am <sub>5</sub>
0.2921	Rb <sub>2</sub> (Fe <sub>2</sub> Ti <sub>6</sub> ) <sub>16</sub>	0.6617	Li <sub>4</sub> Np <sub>5</sub>
0.2923	Rb <sub>2</sub> (CuTi <sub>7</sub> ) <sub>16</sub>	0.6617	Li <sub>4</sub> U <sub>5</sub>
0.2924	K <sub>2</sub> (NiTi <sub>7</sub> ) <sub>16</sub>	0.6621	Li <sub>4</sub> Pu <sub>5</sub>
0.2926	K <sub>2</sub> (Fe <sub>2</sub> Ti <sub>6</sub> ) <sub>16</sub>	0.6796	NH <sub>4</sub> Sb <sub>4</sub> F <sub>13</sub>
0.2926	K <sub>2</sub> (ZnTi <sub>7</sub> ) <sub>16</sub>	0.6812	RbSb <sub>4</sub> F <sub>13</sub>
0.2927	K <sub>2</sub> (Ga <sub>2</sub> Ti <sub>6</sub> ) <sub>16</sub>	0.6832	TlSb <sub>4</sub> F <sub>13</sub>
0.2928	K <sub>2</sub> (Al <sub>2</sub> Ti <sub>6</sub> ) <sub>16</sub>	0.6854	UF <sub>5</sub>
0.2928	K <sub>2</sub> (MgTi <sub>7</sub> ) <sub>16</sub>	0.7039	CsSb <sub>4</sub> F <sub>13</sub>
0.2932	(K, Ba) <sub>1.33</sub> (Ti, Fe) <sub>8</sub> O <sub>16</sub>	0.7057	Ce <sub>5</sub> Mg <sub>4</sub> O <sub>2</sub>
0.2934	K <sub>2</sub> (CoTi <sub>7</sub> ) <sub>16</sub>	0.7453	Na <sub>2</sub> (Ti, Fe)(OH)Si <sub>4</sub> O <sub>10</sub>
0.2937	K <sub>2</sub> (CuTi <sub>7</sub> ) <sub>16</sub>	0.9302	AgCl <sub>3</sub>
0.2954	Ba <sub>x</sub> (Ti <sub>8-x</sub> Mg <sub>x</sub> ) <sub>16</sub>	0.9650	Ce <sub>6</sub> O <sub>4</sub> (OH) <sub>4</sub> (SO <sub>4</sub> ) <sub>6</sub>
0.3415	As <sub>4</sub> Mo <sub>5</sub>	0.9661	U <sub>6</sub> O <sub>4</sub> (OH) <sub>4</sub> (SO <sub>4</sub> ) <sub>6</sub>
0.3448	Nb <sub>5</sub> Sb <sub>4</sub>	1.2268	ThH <sub>2</sub>
0.3454	As <sub>4</sub> (Ti, W) <sub>5</sub>	1.2572	HfD <sub>2</sub>
0.3460	Sb <sub>4</sub> Ta <sub>5</sub>	1.2639	ZrH <sub>2</sub>
0.3498	Nb <sub>5</sub> Se <sub>4</sub>	1.2699	HfH <sub>2</sub>
0.3635	Nb <sub>5</sub> Te <sub>4</sub>	1.6978	K <sub>2</sub> SO <sub>2</sub> (OH) <sub>4</sub>
Organic			
0.2479	C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>	1.0161	(CH <sub>3</sub> ) <sub>2</sub> CN(CH <sub>3</sub> ) <sub>2</sub> •ClO <sub>4</sub>
0.4498	[(CH <sub>3</sub> ) <sub>3</sub> As•PdCl <sub>2</sub> ] <sub>2</sub>	1.2899	[(CH <sub>3</sub> ) <sub>4</sub> N] <sub>2</sub> UO <sub>2</sub> Cl <sub>4</sub>
0.450	[(CH <sub>3</sub> ) <sub>3</sub> As•PdBr <sub>2</sub> ] <sub>2</sub>	1.2904	[(C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> N] <sub>2</sub> PuO <sub>2</sub> Cl <sub>4</sub>
0.5850	Sr(OOC•CO <sub>2</sub> ) <sub>2</sub> •2.17H <sub>2</sub> O	1.2928	[(CH <sub>3</sub> ) <sub>4</sub> N] <sub>2</sub> PuO <sub>2</sub> Cl <sub>4</sub>
0.5944	CaC <sub>2</sub> O <sub>4</sub> •2H <sub>2</sub> O	1.420	[(CH <sub>3</sub> ) <sub>4</sub> N] <sub>2</sub> SiF <sub>6</sub>
0.7228	C <sub>44</sub> H <sub>28</sub> N <sub>4</sub> Zn•2H <sub>2</sub> O		

$\frac{4}{m}$	I4 <sub>1</sub> /a $C_{4h}^6$	No. 88	Inorganic - 138 Organic - 34
Inorganic			
0.2907	(Mg, Ca, OH, H <sub>2</sub> O) <sub>2</sub> (Ti, Cr, Si) <sub>8</sub> O <sub>16</sub>	1.9892	K <sub>3</sub> UF <sub>7</sub>
0.2988	Ba <sub>4</sub> (Ti, Nb) <sub>8</sub> Cl <sub>16</sub> (Si <sub>4</sub> O <sub>12</sub> )	2.0565	LiLuF <sub>4</sub>
0.3000	Ba <sub>4</sub> Ti <sub>7</sub> NbSi <sub>4</sub> O <sub>28</sub> Cl	2.0603	LiYbF <sub>4</sub>
0.4370	Nb <sub>2</sub> O <sub>2</sub>	2.0635	LiYbF <sub>4</sub>
0.4371	Li <sub>7</sub> Th <sub>6</sub> F <sub>31</sub>	2.0660	LiTmF <sub>4</sub>
0.4398	LiUF <sub>5</sub>	2.0687	CaZnF <sub>4</sub>
0.4403	LiNpF <sub>5</sub>	2.0728	LiErF <sub>4</sub>
0.4408	LiAmF <sub>5</sub>	2.0754	LiYF <sub>4</sub>
0.4416	LiPuF <sub>5</sub>	2.0773	LiHoF <sub>4</sub>
0.4418	LiCmF <sub>5</sub>	2.0798	LiYF <sub>4</sub>
0.4926	Na <sub>4</sub> Ge <sub>9</sub> O <sub>20</sub>	2.0829	LiDyF <sub>4</sub>
0.4929	Na <sub>4</sub> Ge <sub>9</sub> O <sub>20</sub>	2.0833	LiHoF <sub>4</sub>
0.5252	GaMg	2.0875	LiDyF <sub>4</sub>
0.6465	CuN <sub>3</sub>	2.0942	LiTbF <sub>4</sub>
0.8211	Al <sub>21</sub> Pt <sub>8</sub>	2.1019	LiGdF <sub>4</sub>
0.9898	BiNa <sub>5</sub> (WO <sub>4</sub> ) <sub>4</sub>	2.1098	LiEuF <sub>4</sub>
0.9953	LaNa <sub>5</sub> (WO <sub>4</sub> ) <sub>4</sub>	2.1105	(Y, Yb)NbO <sub>4</sub>
1.0066	BiNa <sub>5</sub> (MoO <sub>4</sub> ) <sub>4</sub>	2.1113	LiGdF <sub>4</sub>
1.0529	KAlSi <sub>2</sub> O <sub>6</sub>	2.1152	LiEuF <sub>4</sub>
1.0541	KAlSi <sub>2</sub> O <sub>6</sub>	2.1210	HoTaO <sub>4</sub>
1.0623	KAlSi <sub>2</sub> O <sub>6</sub>	2.1250	TmNbO <sub>4</sub>
1.6727	Co(NH <sub>3</sub> ) <sub>3</sub> (NO <sub>2</sub> ) <sub>2</sub> Cl	2.1259	YbNbO <sub>4</sub>
1.9833	K <sub>3</sub> UO <sub>2</sub> F <sub>5</sub>	2.1356	YNbO <sub>4</sub>



I4<sub>1</sub>/a C<sub>4h</sub><sup>6</sup> No. 88 (continued)

## Inorganic (continued)

2.1373	LuTi <sub>0.5</sub> W <sub>0.5</sub> θ <sub>4</sub>	2.1955	AmGeθ <sub>4</sub>
2.1397	SrZnF <sub>4</sub>	2.1958	LaNa(Moθ <sub>4</sub> ) <sub>2</sub>
2.1402	SmNbθ <sub>4</sub>	2.1965	KIθ <sub>4</sub>
2.1441	HoNbθ <sub>4</sub>	2.1971	BiLi(Moθ <sub>4</sub> ) <sub>2</sub>
2.1463	ErTi <sub>0.5</sub> W <sub>0.5</sub> θ <sub>4</sub>	2.1990	LaLi(Moθ <sub>4</sub> ) <sub>2</sub>
2.1482	HoTi <sub>0.5</sub> W <sub>0.5</sub> θ <sub>4</sub>	2.1994	SmTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>
2.1491	GdNbθ <sub>4</sub>	2.2017	SrWθ <sub>4</sub>
2.1538	TbTi <sub>0.5</sub> W <sub>0.5</sub> θ <sub>4</sub>	2.2025	RbIθ <sub>4</sub>
2.1539	NH <sub>4</sub> Iθ <sub>4</sub>	2.2028	NdTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>
2.1542	DyTi <sub>0.5</sub> W <sub>0.5</sub> θ <sub>4</sub>	2.2043	NH <sub>4</sub> Reθ <sub>4</sub>
2.1546	GdTi <sub>0.5</sub> W <sub>0.5</sub> θ <sub>4</sub>	2.2044	PuGeθ <sub>4</sub>
2.1558	HfGeθ <sub>4</sub>	2.2051	NpGeθ <sub>4</sub>
2.1562	NdNbθ <sub>4</sub>	2.2056	PrTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>
2.1578	CaWθ <sub>4</sub>	2.2070	PbWθ <sub>4</sub>
2.1626	NdTαθ <sub>4</sub>	2.2081	UGeθ <sub>4</sub>
2.1628	EuTi <sub>0.5</sub> W <sub>0.5</sub> θ <sub>4</sub>	2.2109	KLa(Wθ <sub>4</sub> ) <sub>2</sub>
2.1644	CdMoθ <sub>4</sub>	2.2117	CeTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>
2.1650	SmTi <sub>0.5</sub> W <sub>0.5</sub> θ <sub>4</sub>	2.2126	UGeθ <sub>4</sub>
2.1656	HfGeθ <sub>4</sub>	2.2135	CeGeθ <sub>4</sub>
2.1681	ZrGeθ <sub>4</sub>	2.2149	BiK(Moθ <sub>4</sub> ) <sub>2</sub>
2.1681	CaWθ <sub>4</sub>	2.2160	LuVθ <sub>4</sub>
2.1698	CaWθ <sub>4</sub>	2.2167	CeK(Wθ <sub>4</sub> ) <sub>2</sub>
2.1700	ZrGeθ <sub>4</sub>	2.2249	SrMoθ <sub>4</sub>
2.1709	CeNbθ <sub>4</sub>	2.2262	KReθ <sub>4</sub>
2.1729	NdTi <sub>0.5</sub> W <sub>0.5</sub> θ <sub>4</sub>	2.2277	AgReθ <sub>4</sub>
2.1740	LuTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>	2.2288	PaGeθ <sub>4</sub>
2.1740	CdMoθ <sub>4</sub>	2.2291	PbMoθ <sub>4</sub>
2.1744	YbTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>	2.2310	PbMoθ <sub>4</sub>
2.1759	YTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>	2.2331	HoVθ <sub>4</sub>
2.1761	TmTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>	2.2351	KLa(Moθ <sub>4</sub> ) <sub>2</sub>
2.1762	LaNa(Wθ <sub>4</sub> ) <sub>2</sub>	2.2379	AgIθ <sub>4</sub>
2.1777	Ca(W <sub>2</sub> Mo)θ <sub>4</sub>	2.2416	NaIθ <sub>4</sub>
2.1777	Ce <sub>2</sub> (Wθ <sub>4</sub> ) <sub>3</sub>	2.2445	ThGeθ <sub>4</sub>
2.1792	CeNa(Wθ <sub>4</sub> ) <sub>2</sub>	2.2518	BaWθ <sub>4</sub>
2.1798	LaLi(Wθ <sub>4</sub> ) <sub>2</sub>	2.2555	ErAsθ <sub>4</sub>
2.1808	ErTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>	2.2611	YbAsθ <sub>4</sub>
2.1817	HoTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>	2.2690	RbReθ <sub>4</sub>
2.1842	TbTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>	2.2956	BaMoθ <sub>4</sub>
2.1853	NaReθ <sub>4</sub>	2.3031	BiAsθ <sub>4</sub>
2.1866	DyTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>	2.3138	TlReθ <sub>4</sub>
2.1874	CaMoθ <sub>4</sub>	2.3150	Kθ <sub>3</sub> N
2.1878	Ca(Mo <sub>2</sub> W)θ <sub>4</sub>	2.3161	KRuθ <sub>4</sub>
2.1898	LaNbθ <sub>4</sub>	2.3608	KCr(θ <sub>3</sub> F)
2.1932	GdTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>	2.5188	CsSθ <sub>3</sub> F
2.1933	BiNa(Moθ <sub>4</sub> ) <sub>2</sub>	2.5372	CsCrθ <sub>3</sub> F
2.1940	EuTi <sub>0.5</sub> Mo <sub>0.5</sub> θ <sub>4</sub>	3.5968	K <sub>4</sub> Fe(CN) <sub>6</sub> •3H <sub>2</sub> θ

## Organic

0.3616	CθCl <sub>2</sub>	1.3600	Ni(CH <sub>3</sub> C <sub>5</sub> H <sub>4</sub> N) <sub>4</sub> (SCN) <sub>2</sub> •0.69C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>
0.4091	[PN(CH <sub>3</sub> ) <sub>2</sub> ] <sub>4</sub>	1.3730	Ni(CH <sub>3</sub> C <sub>5</sub> H <sub>4</sub> N) <sub>4</sub> (SCN) <sub>2</sub> •0.67C <sub>6</sub> H <sub>5</sub> Nθ <sub>2</sub>
0.4242	[(CH <sub>3</sub> ) <sub>2</sub> Siθ] <sub>4</sub>	1.3751	Co(CH <sub>3</sub> C <sub>5</sub> H <sub>4</sub> N) <sub>4</sub> (SCN) <sub>2</sub> •0.67C <sub>2</sub> H <sub>5</sub> Nθ <sub>2</sub>
0.4817	C <sub>20</sub> H <sub>36</sub> B <sub>4</sub> N <sub>8</sub> S <sub>4</sub>	1.3873	Co(CH <sub>3</sub> C <sub>5</sub> H <sub>4</sub> N) <sub>4</sub> (SCN) <sub>2</sub> •0.57C <sub>6</sub> H <sub>6</sub>
0.4867	CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> Sθ <sub>2</sub> NH <sub>2</sub>	1.7525	FeCl <sub>2</sub> (CH <sub>3</sub> SθCH <sub>3</sub> ) <sub>4</sub> •FeCl <sub>4</sub>
0.517	Hg(S•C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub>	1.8949	NH <sub>4</sub> Uθ <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> Cθθ) <sub>3</sub>
0.5341	CH <sub>2</sub> θH•(CHθR) <sub>2</sub> •CH <sub>2</sub> θH	1.9095	TlUθ <sub>2</sub> (CH <sub>3</sub> Cθθ) <sub>3</sub>
0.545	[(C <sub>6</sub> H <sub>5</sub> )Al•N(C <sub>6</sub> H <sub>5</sub> )] <sub>4</sub>	1.9921	Rh(Uθ <sub>2</sub> )(CH <sub>3</sub> Cθθ) <sub>3</sub>
0.5463	C <sub>8</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>8</sub>	2.0393	[(CH <sub>3</sub> ) <sub>3</sub> C•Cθ:CH•Cθ•C(CH <sub>3</sub> ) <sub>3</sub> ] <sub>2</sub> Zn
0.5470	C <sub>8</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>8</sub>	2.0497	[(CH <sub>3</sub> ) <sub>3</sub> C•Cθ:CH•Cθ•C(CH <sub>3</sub> ) <sub>3</sub> ] <sub>2</sub> Co
0.7084	C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> θ <sub>2</sub> Pd	2.165	AgUθ <sub>2</sub> (CH <sub>3</sub> •Cθθ) <sub>3</sub> •xH <sub>2</sub> θ
0.9487	LiBr•4(CH <sub>3</sub> CθNHCH <sub>3</sub> )	2.3596	Pt(C <sub>2</sub> H <sub>4</sub> )NH <sub>3</sub> •Br <sub>2</sub>
0.9617	LiCl•4(CH <sub>3</sub> CθNHCH <sub>3</sub> )	3.1223	Zn(C <sub>5</sub> H <sub>4</sub> N•C <sub>5</sub> H <sub>3</sub> N•C <sub>5</sub> H <sub>4</sub> N) <sub>2</sub> Sθ <sub>4</sub> •4H <sub>2</sub> θ
1.3338	Ni(CH <sub>3</sub> C <sub>5</sub> H <sub>4</sub> N) <sub>4</sub> (SCN) <sub>2</sub> •0.53C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>	3.1578	Sm(C <sub>10</sub> H <sub>13</sub> N <sub>2</sub> θ <sub>8</sub> )•H <sub>2</sub> θ
1.3568	Ni(CH <sub>3</sub> C <sub>5</sub> H <sub>4</sub> N) <sub>4</sub> (SCN) <sub>2</sub> •0.83C <sub>6</sub> H <sub>6</sub>	3.4948	[As(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> ] <sub>2</sub> Co(CF <sub>3</sub> Cθθ) <sub>4</sub>
1.3583	Ni(CH <sub>3</sub> C <sub>5</sub> H <sub>4</sub> N) <sub>4</sub> (SCN) <sub>2</sub> •0.67C <sub>2</sub> H <sub>5</sub> Nθ <sub>2</sub>	3.4965	[(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> As] <sub>2</sub> Co(θ <sub>2</sub> CCF <sub>3</sub> ) <sub>4</sub>
1.3594	Ni(CH <sub>3</sub> C <sub>5</sub> H <sub>4</sub> N) <sub>4</sub> (SCN) <sub>2</sub> •0.53CH <sub>3</sub> θH	3.596	K <sub>4</sub> Fe(CN) <sub>6</sub> •3H <sub>2</sub> θ

4 2 2	P4 <sub>2,1</sub> 2	D <sub>4</sub> <sup>2</sup>	No. 90	Inorganic - 2 Organic - 1
Inorganic				
0.6918	Np	1.4280	K <sub>2</sub> SnBr <sub>6</sub>	
Organic				
0.937	(C <sub>6</sub> H <sub>10</sub> <sup>δ</sup> <sub>5</sub> •C <sub>3</sub> H <sub>7</sub> <sup>δ</sup> H) <sub>8</sub>			
4 2 2	P4 <sub>1,22</sub>	D <sub>4</sub> <sup>3</sup>	No. 91 (includes P4 <sub>3,22</sub> No. 95)	Inorganic - 4 Organic - 4
Inorganic				
1.0589	Al <sub>2</sub> C <sub>12</sub> <sup>δ</sup> <sub>12</sub> •18H <sub>2</sub> <sup>δ</sup>	1.3771	Na <sub>2</sub> S•9H <sub>2</sub> <sup>δ</sup>	
1.3750	Na <sub>2</sub> Se•9H <sub>2</sub> <sup>δ</sup>	1.4013	Zn <sub>2</sub> Ti <sup>δ</sup> <sub>4</sub>	
Organic				
1.0589	Al <sub>2</sub> C <sub>12</sub> <sup>δ</sup> <sub>12</sub> •18H <sub>2</sub> <sup>δ</sup>	2.805	C <sub>5</sub> H <sub>4</sub> <sup>δ</sup> <sub>4</sub> N <sub>4</sub>	
1.6820	[Co(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>3</sub> ]Br <sub>3</sub> •H <sub>2</sub> <sup>δ</sup>	3.8471	C <sub>36</sub> H <sub>45</sub> N <sup>δ</sup> <sub>17</sub> •CHCl <sub>3</sub>	
4 2 2	P4 <sub>1,2,1</sub> 2	D <sub>4</sub> <sup>4</sup>	No. 92 (includes P4 <sub>3,2,1</sub> 2 No. 96)	Inorganic - 33 Organic - 37
Inorganic				
0.9788	Fe <sub>44</sub> Si <sub>29.5</sub> V <sub>26.5</sub>	1.8252	Si <sub>4</sub> Zr <sub>5</sub>	
1.0000	H <sub>2</sub> <sup>δ</sup>	1.9704	H <sub>2</sub> <sup>δ</sup> <sub>2</sub>	
1.1540	Si <sup>δ</sup> <sub>2</sub>	2.4263	(U <sup>δ</sup> <sub>2</sub> •xH <sub>2</sub> <sup>δ</sup> )(U <sup>δ</sup> <sub>2</sub> As <sup>δ</sup> <sub>4</sub> ) <sub>2</sub>	
1.1771	Ge	2.6503	Fe <sub>3</sub> Na(δH) <sub>4</sub> (P <sup>δ</sup> <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> <sup>δ</sup>	
1.2127	LiAl <sup>δ</sup> <sub>2</sub>	2.6566	ZnSe <sup>δ</sup> <sub>4</sub> •6H <sub>2</sub> <sup>δ</sup>	
1.2152	LiAlSi <sup>δ</sup> <sub>2</sub> <sub>6</sub>	2.6642	NiSe <sup>δ</sup> <sub>4</sub> •6H <sub>2</sub> <sup>δ</sup>	
1.2173	LiAl <sup>δ</sup> <sub>2</sub>	2.6818	Al <sub>3</sub> Na(δH) <sub>4</sub> (P <sup>δ</sup> <sub>4</sub> ) <sub>2</sub> •2H <sub>2</sub> <sup>δ</sup>	
1.3129	NaFe <sup>δ</sup> <sub>2</sub>	2.6907	NiS <sup>δ</sup> <sub>4</sub> •6H <sub>2</sub> <sup>δ</sup>	
1.3911	AlB <sub>12</sub>	2.6912	NiS <sup>δ</sup> <sub>4</sub> •6H <sub>2</sub> <sup>δ</sup>	
1.3952	Si <sup>δ</sup> <sub>2</sub>	2.8192	In <sub>5</sub> Br <sub>7</sub>	
1.4055	BeB <sub>6</sub>	2.8244	Cu <sub>2</sub> S	
1.4057	AlB <sub>12</sub>	3.1741	As <sub>6</sub> Ni <sub>11</sub>	
1.5827	Te <sup>δ</sup> <sub>2</sub>	3.6346	P <sub>2</sub> Zn	
1.5901	Te <sup>δ</sup> <sub>2</sub>	3.6594	P <sub>2</sub> Zn	
1.7311	(Fe, Mn)Fe <sub>2</sub> (δH) <sub>2</sub> (P <sup>δ</sup> <sub>4</sub> ) <sub>2</sub>	3.6785	P <sub>2</sub> Zn	
1.8172	Ge <sub>4</sub> Zr <sub>5</sub>	3.7311	CdP <sub>2</sub>	
1.8221	Hf <sub>5</sub> Si <sub>4</sub>			
Organic				
0.9964	Cu[SC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>3</sub> I	3.4026	Se(C <sub>6</sub> H <sub>5</sub> S <sub>2</sub> <sup>δ</sup> <sub>2</sub> ) <sub>2</sub>	
1.0283	Cu[SC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>3</sub> Cl	3.5124	C <sub>24</sub> H <sub>40</sub> <sup>δ</sup> <sub>4</sub> •C <sub>2</sub> H <sub>5</sub> <sup>δ</sup> H	
1.0349	Cu[SC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>3</sub> Br	3.7011	C <sub>15</sub> H <sub>18</sub> N <sub>2</sub> <sup>δ</sup> <sub>5</sub>	
1.3808	Ca <sub>2</sub> Pb(CH <sub>3</sub> CH <sub>2</sub> C <sup>δ</sup> <sub>6</sub> ) <sub>6</sub>	3.7557	Cl <sub>2</sub> C <sub>6</sub> H <sub>2</sub> <sup>δ</sup> <sub>2</sub>	
1.3846	Ca <sub>2</sub> Sr(CH <sub>3</sub> CH <sub>2</sub> C <sup>δ</sup> <sub>6</sub> ) <sub>6</sub>	3.771	(C <sub>21</sub> H <sub>22</sub> <sup>δ</sup> <sub>6</sub> N) <sub>2</sub> •Cu•6H <sub>2</sub> <sup>δ</sup>	
1.4461	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> <sup>δ</sup>	3.8190	Se(Se•CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> S <sup>δ</sup> <sub>2</sub> ) <sub>2</sub>	
1.6814	[Co(NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>3</sub> ]Br <sub>3</sub> •H <sub>2</sub> <sup>δ</sup>	3.831	C <sub>14</sub> H <sub>14</sub> <sup>δ</sup> <sub>4</sub> S <sub>5</sub>	
1.9118	C <sub>22</sub> H <sub>28</sub> Br <sub>2</sub> N <sub>4</sub>	3.8441	Se(S•CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> S <sup>δ</sup> <sub>2</sub> ) <sub>2</sub>	
2.0466	C <sub>21</sub> H <sub>21</sub> N <sup>δ</sup> <sub>4</sub> •CH <sub>3</sub> I	3.8655	Te(S•CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> S <sup>δ</sup> <sub>2</sub> ) <sub>2</sub>	
2.3340	[CLRh(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> ] <sub>2</sub>	3.8930	C <sub>15</sub> H <sub>18</sub> N <sub>2</sub> <sup>δ</sup> <sub>5</sub>	
2.381	C <sub>22</sub> H <sub>26</sub> N <sub>4</sub> PtCl <sub>6</sub>	4.0385	Zn(C <sub>6</sub> H <sub>8</sub> N <sub>3</sub> <sup>δ</sup> <sub>2</sub> ) <sub>2</sub> •2H <sub>2</sub> <sup>δ</sup>	
2.396	C <sub>4</sub> H <sub>2</sub> N <sub>2</sub> <sup>δ</sup> <sub>4</sub>	4.1272	Cd(C <sub>6</sub> H <sub>8</sub> N <sub>3</sub> <sup>δ</sup> <sub>2</sub> ) <sub>2</sub> •2H <sub>2</sub> <sup>δ</sup>	
2.5417	Al(δC <sub>3</sub> H <sub>7</sub> ) <sub>3</sub>	4.590	C <sub>7</sub> H <sub>14</sub> <sup>δ</sup> <sub>6</sub> •0.5H <sub>2</sub> <sup>δ</sup>	
2.7986	[HNC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>2</sub> •H <sub>2</sub> C <sup>δ</sup> <sub>3</sub>	4.6934	[C <sub>4</sub> H <sub>4</sub> (C <sup>δ</sup> <sub>6</sub> CH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub>	
2.817	(N <sup>δ</sup> <sub>2</sub> ) <sub>3</sub> (C <sub>6</sub> H <sub>2</sub> ) <sub>1</sub>	4.892	C <sub>4</sub> H <sub>8</sub> I <sub>2</sub> S <sub>3</sub>	
3.0100	(NH <sub>3</sub> •CH <sub>2</sub> •CH <sub>2</sub> •NH <sub>3</sub> ) <sub>3</sub> S <sup>δ</sup> <sub>4</sub>	5.7210	C <sub>30</sub> H <sub>30</sub> Br <sub>2</sub> N <sub>4</sub> <sup>δ</sup> <sub>4</sub>	
3.0444	Ni[SC(NH <sub>2</sub> ) <sub>2</sub> ] <sub>6</sub> (Cl <sup>δ</sup> <sub>4</sub> ) <sub>2</sub>	6.9518	C <sub>23</sub> H <sub>28</sub> N <sub>2</sub> <sup>δ</sup> <sub>6</sub> •CH <sub>3</sub> I	
3.226	(SC <sub>2</sub> H <sub>3</sub> NH <sub>2</sub> C <sup>δ</sup> <sub>6</sub> H) <sub>2</sub>	7.3130	C <sub>33</sub> H <sub>31</sub> IN <sub>2</sub> <sup>δ</sup> <sub>6</sub> •C <sub>3</sub> H <sub>6</sub> <sup>δ</sup>	
3.397	C <sub>12</sub> H <sub>10</sub> <sup>δ</sup> <sub>4</sub> S <sub>5</sub>			
4 2 2	P4 <sub>2,22</sub>	D <sub>4</sub> <sup>5</sup>	No. 93	Inorganic - 1 Organic - 0
Inorganic				
2.5244	Ba(U <sup>δ</sup> <sub>2</sub> ) <sub>2</sub> (P <sup>δ</sup> <sub>4</sub> ) <sub>2</sub> •10H <sub>2</sub> <sup>δ</sup>			

P4<sub>2</sub>22 D<sub>4</sub><sup>5</sup> No. 93 (continued)

Organic

.....

4 2 2

P4<sub>2</sub>2<sub>1</sub>2 D<sub>4</sub><sup>6</sup> No. 94

Inorganic - 7  
Organic - 4

Inorganic

0.5180 MoNi 1.0485 Li<sub>3</sub>PaF<sub>8</sub>  
0.6765 Hg<sub>3</sub>S<sub>2</sub>Br<sub>2</sub> 1.0788 Hf<sub>2</sub>OF<sub>6</sub>  
0.7906 Sc<sub>4</sub>(P<sub>2</sub>O<sub>7</sub>)<sub>3</sub> 1.0884 Hf<sub>2</sub>OF<sub>6</sub>•H<sub>2</sub>O  
0.7975 Al<sub>5</sub>(Na,K)(Ca,RE,Th)<sub>2</sub>[(SiO<sub>4</sub>)(PO<sub>4</sub>)(SO<sub>4</sub>)<sub>4</sub>]  
(OH)<sub>6</sub>•6•5.6H<sub>2</sub>O

Organic

0.3715 C<sub>22</sub>H<sub>16</sub> 1.874 C<sub>11</sub>H<sub>14</sub>N<sub>2</sub>O<sub>3</sub>  
0.7175 CsO<sub>5</sub>C<sub>4</sub>(CH<sub>3</sub>)<sub>8</sub> 2.2233 MgBr<sub>2</sub>•4C<sub>4</sub>H<sub>8</sub>O

4 2 2

P4<sub>3</sub>22 D<sub>4</sub><sup>7</sup> No. 95 (see No. 91)

.....

4 2 2

P4<sub>3</sub>2<sub>1</sub>2 D<sub>4</sub><sup>8</sup> No. 96 (see No. 92)

.....

4 2 2

I4<sub>1</sub>22 D<sub>4</sub><sup>9</sup> No. 97

Inorganic - 5  
Organic - 0

Inorganic

3.1634 Li<sub>2</sub>HgO<sub>2</sub> 3.5561 K<sub>2</sub>HgO<sub>2</sub>  
3.3356 Cs<sub>2</sub>HgO<sub>2</sub> 3.8947 Na<sub>2</sub>HgO<sub>2</sub>  
3.4358 Rb<sub>2</sub>HgO<sub>2</sub>

Organic

.....

4 2 2

I4<sub>1</sub>22 D<sub>4</sub><sup>10</sup> No. 98

Inorganic - 7  
Organic - 3

Inorganic

0.5402 N<sub>2</sub>O<sub>3</sub> 3.4204 PTa  
0.5878 As<sub>2</sub>Cd 3.4226 NbP  
1.0957 Zr(OH)<sub>2</sub>(MoO<sub>3</sub>OH)<sub>2</sub> 7.3398 Ge<sub>1.7</sub>Mo  
2.3855 Fe<sub>1.75</sub>OHPO<sub>4</sub>

Organic

1.794 KUO<sub>2</sub>(CH<sub>3</sub>COO)<sub>3</sub> 2.001 NH<sub>4</sub>VO<sub>2</sub>(CH<sub>3</sub>COO)<sub>3</sub>  
1.980 KUO<sub>2</sub>(CH<sub>3</sub>COO)<sub>3</sub>

4 m m

P4mm C<sub>4v</sub><sup>1</sup> No. 99

Inorganic - 4  
Organic - 1

Inorganic

0.9359 CuPb<sub>2</sub>(OH)<sub>4</sub>Cl<sub>2</sub> 1.0635 PbTiO<sub>3</sub>  
0.9365 CuPb<sub>2</sub>(OH)<sub>4</sub>Cl<sub>2</sub> 1.3873 BiNa

Organic

0.5851 K<sub>2</sub>Pt(CN)<sub>5</sub>•3H<sub>2</sub>O

4 mm	P4bm	$C_{4v}^2$	No. 100	Inorganic - 3 Organic - 0
-----				
Inorganic				
0.3198	$Ba_6Ti_2Nb_8O_{30}$		0.8711	$NH_4NO_3$
0.7071	$LiCl \cdot H_2O$			
Organic				
.....				
4 mm	P4 <sub>2</sub> cm	$C_{4v}^3$	No. 101	Inorganic - 0 Organic - 0
-----				
.....				
4 mm	P4 <sub>2</sub> nm	$C_{4v}^4$	No. 102	Inorganic - 4 Organic - 1
-----				
Inorganic				
0.5192	$Re_3V$		0.6750	$[(NH_3)_5Co-O_2-Co(NH_3)_5](NO_3)_5$
0.5295	U		0.7089	$[(NH_3)_5Co]_2NH_2(NO_3)_5$
Organic				
0.3245	$C_6H_{12}O_2Se$			
-----				
4 mm	P4cc	$C_{4v}^5$	No. 103	Inorganic - 1 Organic - 0
-----				
Inorganic				
1.0453	$TaTe_4$			
Organic				
.....				
4 mm	P4nc	$C_{4v}^6$	No. 104	Inorganic - 0 Organic - 1
-----				
Inorganic				
.....				
Organic				
1.557	$[N(CH_3)_2(C_2H_5)_2]_2SnCl_6$			
-----				
4 mm	P4 <sub>2</sub> mc	$C_{4v}^7$	No. 105	Inorganic - 0 Organic - 0
-----				
.....				
4 mm	P4 <sub>2</sub> bc	$C_{4v}^8$	No. 106	Inorganic - 0 Organic - 1
-----				
Inorganic				
.....				
Organic				
0.8791	$C_3H_2S_3$			

4 m m	I4mm	$C_{4v}^9$	No. 107	Inorganic - 7 Organic - 2
Inorganic				
0.7514	$B_5H_9$		1.0071	$Au_3Cd$
0.7605	$Co_5Ge_7$		1.0753	$H_3NB_3H_7$
0.9374	HCN		3.1998	$BiCd_2Br$
0.9606	$H_3N \cdot BH_3$			
Organic				
0.4059	$(Pt(C_2H_5NH_2)_4Cl_2)(Pt(C_2H_5NH_2)_4)Cl_4 \cdot 4H_2O$		0.937	HCN
4 m m	I4cm	$C_{4v}^{10}$	No. 108	Inorganic - 2 Organic - 0
Inorganic				
0.6151	$SrBr_2$		1.3479	$KCuF_3$
Organic				
.....				
4 m m	$I4_1md$	$C_{4v}^{11}$	No. 109	Inorganic - 5 Organic - 0
Inorganic				
2.2036	$AgYbS_2$		3.4127	$NbP$
3.3826	$AsNb$		3.4170	$PTa$
3.3913	$AsTa$			
Organic				
.....				
4 m m	$I4_1cd$	$C_{4v}^{12}$	No. 110	Inorganic - 2 Organic - 2
Inorganic				
0.6784	$Be(BH_4)_2$		1.0834	$Li_2B_4O_7$
Organic				
3.5369	$C_{10}H_7N$		4.077	$C_9H_4O_3$
$\bar{4} 2 m$ $\bar{4} m 2$	$P\bar{4}2m$	$D_{2d}^1$	No. 111	Inorganic - 4 Organic - 0
Inorganic				
1.0000	$CdIn_2Se_4$		1.0161	$Li_3MnP_2$
1.0090	$Cu_2HgI_4$		1.0824	$Na_2Al_2O_4$
Organic				
.....				
$\bar{4} 2 m$ $\bar{4} m 2$	$P\bar{4}2c$	$D_{2d}^2$	No. 112	Inorganic - 2 Organic - 1
Inorganic				
1.0792	$Pd_4Se$		1.0930	$Pd_4S$
Organic				
1.1300	$C_{28}H_{28}Si$			

$\bar{4} 2 m$ $\bar{4} m 2$	$P\bar{4}2_1m$	$D_{2d}^3$	No. 113	Inorganic - 28 Organic - 4
Inorganic				
0.5969	$NH_4ClO_2$		0.6602	$CaPrAl_3O_7$
0.6134	$(PbCl_4)(ICl_2)$		0.6616	$CaPrGa_3O_7$
0.6227	$Sr_2FeSi_2O_7$		0.6620	$CaLaAl_3O_7$
0.6355	$Sr_2MnSi_2O_7$		0.6620	$CaNdGa_3O_7$
0.6373	$Ca_2ZnSi_2O_7$		0.6622	$CaSmGa_3O_7$
0.6398	$Ca_2MgSi_2O_7$		0.6632	$Ca_2Al_2Si_2O_7$
0.6434	$Ba_2FeSi_2O_7$		0.6650	$CaLaGa_3O_7$
0.6442	$(Ca,Na)_2(Mg,Al)(Si,Al)_2O_7$		0.6680	$Cu_3Se_2$
0.6462	$Ba_2MnSi_2O_7$		0.6693	$LiNa_2Be_2F_7$
0.6463	$Sr_2ZnSi_2O_7$		0.6743	$Ca_2BeSi_2O_7$
0.6554	$CaYAl_3O_7$		0.6813	$Ba_2Al_4Si_6O_{20} \cdot 8H_2O$
0.6563	$Pb_2ZnSi_2O_7$		0.6908	$Ca_2MgSi_2O_7$
0.6576	$CaSmAl_3O_7$		0.7082	$NH_4Cu(NH_3)_5(ClO_4)_3$
0.6599	$Ca_2Al_2Si_2O_7$		0.8451	$Cs_2(UO_2)_2(SO_4)_3$
Organic				
0.5137	$[(CH_3)_3SO]ClO_4$		0.8324	$OC(NH_2)_2$
0.6318	$N(CH_3)_4ICl_2$		0.8759	$(C_4H_6)_2RhCl$

$\bar{4} 2 m$ $\bar{4} m 2$	$P\bar{4}2_1c$	$D_{2d}^4$	No. 114	Inorganic - 9 Organic - 29
Inorganic				
0.4500	$ZrOCl_2 \cdot 8H_2O$		0.7508	$NH_4BeAsO_4$
0.4504	$ZrOBr_2 \cdot 8H_2O$		0.7533	$Ag_2(NH_3)_4SO_4$
0.4676	$(NSF)_4$		1.1756	$P_2S_6Br_2$
0.5479	$(SeO_3)_4$		2.0000	$Cu_5FeS_4$
0.7469	$NH_4BePO_4$			
Organic				
0.528	$Pb(C_6H_5)_4$		0.8270	$[(CH_3)_3CS]_3SiOS_5H_9$
0.540	$Pb(C_6H_5)_4$		0.8284	$[(CH_3)_3CS]_3SiOS_3H_7$
0.544	$Pb(C_6H_5)_4$		0.8297	$[(CH_3)_3CS]_3SiOS_4H_9$
0.561	$Sn(C_6H_5)_4$		0.830	$GeS_4(C_4H_9)_4$
0.590	$Ge(C_6H_5)_4$		0.830	$SiS_4(C_4H_9)_4$
0.613	$((CH_3)_2SiO)_8$		0.830	$SnS_4(C_4H_9)_4$
0.6193	$[(C_5H_{10}N)PF_2]_4Ni$		0.8321	$C_3H_4N_2O_3S$
0.627	$Si(C_6H_5)_4$		0.9390	$C_4H_4O(OH)_4$
0.6524	$[NaAs(C_6H_5)_2]_4$		1.0976	$(CH)_4S_6$
0.665	$C(C_6H_5)_4$		1.1770	$[Cu(NC \cdot CH_2CH_2CH_2CN)_2]NO_3$
0.6732	$C_8H_{15}N \cdot HBr$		1.336	$C_{10}H_{16}$
0.6918	$C_5H_{10}CuNS_2$		1.3739	$C_3H_5 \cdot Fe(CO)_3NO_3$
0.7143	$C(CH_2ON_2)_4$		1.3802	$C_3H_5 \cdot Fe(CO)_3NO_3$
0.7840	$(C_7H_8CuCl)_4$		1.4363	$Mg_4Br_6O_4(C_4H_{10}O)$
0.8141	$C(SCH_3)_4$			

$\bar{4} m 2$ $\bar{4} 2 m$	$P\bar{4}m2$	$D_{2d}^5$	No. 115	Inorganic - 3 Organic - 0
Inorganic				
0.7014	$Pb_2OF_2$		1.0115	$Ba_{2x}Bi_2(1-x)O_{3-x}$
0.8013	$Ni_3Te_2$			
Organic				
.....				

$\bar{4} m 2$ $\bar{4} 2 m$	$P\bar{4}c2$	$D_{2d}^6$	No. 116	Inorganic - 5 Organic - 0
Inorganic				
1.6064	$Ru_2Sn_3$		3.1823	$Mn_4Si_7$
1.9327	$KTaF_6$		8.1756	$Ga_{17}Rh_{10}$
1.9402	$KNbF_6$			

$P\bar{4}c2$   $D_{2d}^6$  No. 116 (continued)

Organic

.....

$\bar{4} m 2$   
 $4 2 m$

$P\bar{4}b2$   $D_{2d}^7$  No. 117

Inorganic - 2  
Organic - 0

Inorganic

0.7280  $Bi_2\theta_3$

0.7454  $Pb_3\theta_4$

Organic

.....

$\bar{4} m 2$   
 $4 2 m$

$P\bar{4}n2$   $D_{2d}^8$  No. 118

Inorganic - 16  
Organic - 0

Inorganic

0.7829  $ZnSb_2\theta_6$

1.0400  $Ga_3Ru$

0.8032  $\theta s_2Si_3$

1.0400  $Ga_3\theta s$

1.0100  $Ga_3Rh$

1.0500  $FeGa_3$

1.0200  $In_3Rh$

2.4399  $Ga_5Ir_3$

1.0300  $Ga_3Ir$

8.7235  $Mn_{11}Si_{19}$

1.0300  $In_3Ir$

9.0241  $Cr_{11}Ge_{19}$

1.0350  $CoGa_3$

10.6130  $Ge_{23}Mo_{13}$

1.0353  $In_3Ru$

14.1540  $Ge_{31}V_{17}$

Organic

.....

$\bar{4} m 2$   
 $4 2 m$

$I\bar{4}m2$   $D_{2d}^9$  No. 119

Inorganic - 2  
Organic - 0

Inorganic

1.0856  $Li_5NaAl_2F_{12}$

3.8827  $AgTlTe_2$

Organic

.....

$\bar{4} m 2$   
 $4 2 m$

$I\bar{4}c2$   $D_{2d}^{10}$  No. 120

Inorganic - 3  
Organic - 0

Inorganic

1.3404  $BeS\theta_4 \cdot 4H_2\theta$

1.9809  $3Mn_2\theta_3 \cdot MnSi\theta_3$

1.5585  $Eu_3Si\theta_5$

Organic

.....

$\bar{4} m 2$   
 $4 2 m$

$I\bar{4}2m$   $D_{2d}^{11}$  No. 121

Inorganic - 30  
Organic - 5

Inorganic

0.4846  $V_3S$

1.2229  $(NH_4)_3Nb\theta_8$

0.4869  $PW_3$

1.9354  $Cu_2HgGeSe_4$

0.4929  $Mo_3P$

1.9455  $Cu_2CdSnS_4$

0.5044  $Si_3V_5$

1.9547  $Cu_2HgSnS_4$

0.5070  $Nb_5Si_3$

1.9643  $Cu_2FeSnS_4$

1.1316  $Ce_3Ta\theta_8$

1.9673  $Cu_2ZnGeSe_4$

1.1343  $K_3Cr\theta_8$

1.9715  $Cu_3AsS_4$

1.1386  $K_3Cr\theta_8$

1.9728  $Cu_2CdSnSe_4$

1.1418  $Rb_3Ta\theta_8$

1.9732  $Cu_2HgSnSe_4$

1.1593  $K_3Nb\theta_8$

1.9770  $Cu_2ZnSnTe_4$

1.1622  $K_3Ta\theta_8$

1.9783  $Cu_3AsS_4$

I42m D<sub>2d</sub><sup>11</sup> No. 121 (continued)

## Inorganic (continued)

1.9824	Cu <sub>3</sub> (As, Sb)S <sub>4</sub>	2.0000	Cu <sub>3</sub> SbS <sub>4</sub>
1.9929	Cu <sub>2</sub> HgSnTe <sub>4</sub>	2.0000	Cu <sub>2</sub> (Zn, Fe)SnS <sub>4</sub>
1.9960	Cu <sub>2</sub> ZnSnS <sub>4</sub>	2.0004	Cu <sub>2</sub> FeSnSe <sub>4</sub>
1.9961	Cu <sub>2</sub> ZnSnSe <sub>4</sub>	3.9105	La <sub>2</sub> MoO <sub>6</sub>

## Organic

0.6472	NaB(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub>	0.7195	Rb[B(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub> ]
0.7031	KB(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub>	0.7453	CsB(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub>
0.7189	NH <sub>4</sub> B(C <sub>6</sub> H <sub>5</sub> ) <sub>4</sub>		

4 2 m  
4 m 2

I42d D<sub>2d</sub><sup>12</sup> No. 122

Inorganic - 59  
Organic - 8

## Inorganic

0.4540	UF <sub>5</sub>	1.9093	Ag <sub>2</sub> In <sub>2</sub> S <sub>4</sub>
0.7721	P(CN) <sub>3</sub>	1.9162	AgInSe <sub>2</sub>
0.9080	SrH <sub>2</sub> GeO <sub>4</sub>	1.9167	ZnCl <sub>2</sub>
0.9177	Hg(CN) <sub>2</sub>	1.9206	AgInS <sub>2</sub>
0.9194	Hg(CN) <sub>2</sub>	1.9335	P <sub>2</sub> SiZn
0.9338	KH <sub>2</sub> PtO <sub>4</sub>	1.9340	P <sub>2</sub> SiZn
0.9373	KH <sub>2</sub> AsO <sub>4</sub>	1.9419	As <sub>2</sub> SiZn
0.9381	KH <sub>2</sub> PtO <sub>4</sub>	1.9443	CuAlSe <sub>2</sub>
0.9388	KH <sub>2</sub> AsO <sub>4</sub>	1.9567	As <sub>2</sub> CdSn
0.9394	KH <sub>2</sub> AsO <sub>4</sub>	1.9574	CuGaS <sub>2</sub>
0.9604	RhH <sub>2</sub> PtO <sub>4</sub>	1.9589	CuGaS <sub>2</sub>
0.9862	CsH <sub>2</sub> AsO <sub>4</sub>	1.9600	CuGaSe <sub>2</sub>
1.0039	NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub>	1.9607	AgInTe <sub>2</sub>
1.0065	(NH <sub>4</sub> )H <sub>2</sub> PtO <sub>4</sub>	1.9616	CuAlS <sub>2</sub>
1.2859	CuRh <sub>2</sub> O <sub>4</sub>	1.9656	CuFeS <sub>2</sub>
1.2881	CuCr <sub>2</sub> O <sub>4</sub>	1.9665	As <sub>2</sub> GeZn
1.5517	LiBtO <sub>2</sub>	1.9707	GeP <sub>2</sub> Zn
1.5648	LiPN <sub>2</sub>	1.9731	CuGaS <sub>2</sub>
1.6084	SiS <sub>2</sub>	1.9752	CuAlTe <sub>2</sub>
1.6684	GeS <sub>2</sub>	1.9777	Cu <sub>2</sub> Fe <sub>2</sub> S <sub>4</sub>
1.7849	Ag <sub>2</sub> Ga <sub>2</sub> S <sub>4</sub>	1.9870	CuGaTe <sub>2</sub>
1.8016	AgAlS <sub>2</sub>	1.9942	CuTlSe <sub>2</sub>
1.8049	AgAlSe <sub>2</sub>	2.0007	CuInSe <sub>2</sub>
1.8198	AgFeS <sub>2</sub>	2.0010	CuInTe <sub>2</sub>
1.8215	AgGaSe <sub>2</sub>	2.0018	CuTlS <sub>2</sub>
1.8371	CdP <sub>2</sub> Si	2.0025	CuInS <sub>2</sub>
1.8787	CdGeP <sub>2</sub>	2.0047	CuInS <sub>2</sub>
1.8790	AgAlTe <sub>2</sub>	2.0054	CuInS <sub>2</sub>
1.8883	As <sub>2</sub> CdGe	2.0849	(Bi, W) <sub>8-n</sub> O <sub>12</sub>
1.8988	AgGaTe <sub>2</sub>		

## Organic

0.6550	Rh(CO) <sub>2</sub> Cl	0.9215	C <sub>44</sub> H <sub>30</sub> N <sub>4</sub>
0.7721	P(CN) <sub>3</sub>	0.9255	C <sub>44</sub> H <sub>28</sub> N <sub>4</sub> Ni
0.9177	Hg(CN) <sub>2</sub>	0.9270	C <sub>44</sub> H <sub>28</sub> N <sub>4</sub> Pd
0.919	Hg(CN) <sub>2</sub>	0.9308	C <sub>44</sub> H <sub>28</sub> CuN <sub>4</sub>

4 2 2  
m m m

P4/mmm D<sub>4h</sub><sup>1</sup> No. 123

Inorganic - 56  
Organic - 1

## Inorganic

0.5824	K <sub>2</sub> PdCl <sub>4</sub>	0.8453	CdPd
0.5887	K <sub>2</sub> PtCl <sub>4</sub>	0.8644	CuTi <sub>3</sub>
0.5891	K <sub>2</sub> PtBr <sub>4</sub>	0.8730	AgZr <sub>3</sub>
0.5908	K <sub>2</sub> PtCl <sub>4</sub>	0.9092	CuTi
0.5913	(NH <sub>4</sub> ) <sub>2</sub> PdCl <sub>4</sub>	0.9095	HgPt
0.6674	CrSbO <sub>4</sub>	0.9096	CuTi
0.6677	Cu <sub>3</sub> Se <sub>2</sub>	0.9142	CdPt
0.6688	MnSbO <sub>4</sub>	0.9727	CoPt
0.7064	Nb <sub>4</sub> O	0.9879	PbZrO <sub>3</sub>
0.7529	HBtO <sub>2</sub>	0.9934	AgTi
0.8160	PdZn	1.0000	Na <sub>5</sub> Y <sub>9</sub> F <sub>32</sub>
0.8243	RbN <sub>3</sub>	1.0098	BaTiO <sub>3</sub>



P4/mmm  $D_{4h}^1$  No. 123 (continued)

## Inorganic (continued)

1.0117	AlTi	1.4132	$[\text{Fe}(\text{H}_2\text{O})_4\text{Cl}_2]\text{SbCl}_6 \cdot 4\text{H}_2\text{O}$
1.0514	CsNH <sub>2</sub>	1.4847	K <sub>2</sub> NaMnF <sub>6</sub>
1.1291	Pd <sub>1.1</sub> Mg <sub>0.9</sub>	1.7224	NH <sub>4</sub> GaF <sub>4</sub>
1.1485	PbU	1.7293	KAlF <sub>4</sub>
1.2144	Ba(UO <sub>2</sub> ) <sub>2</sub> (F <sub>4</sub> ) <sub>2</sub> · 10H <sub>2</sub> O	1.7320	RbAlF <sub>4</sub>
1.2272	HgPd	1.7645	TlAlF <sub>4</sub>
1.2418	PbTh	1.7692	NH <sub>4</sub> AlF <sub>4</sub>
1.2780	Al <sub>0.89</sub> Mn <sub>1.11</sub>	1.8075	NaAlF <sub>4</sub>
1.3120	FeNNi	1.9106	FeSi <sub>2</sub>
1.3238	AuCu	1.9387	Cr <sub>2</sub> W <sub>6</sub>
1.3238	HgZr	2.0121	Th <sub>0.25</sub> Nb <sub>3</sub>
1.3338	CuZn	2.0189	U(Nb <sub>3</sub> ) <sub>4</sub>
1.3430	HgTi	2.2739	Zr <sub>3</sub> S <sub>2</sub>
1.3529	Mn <sub>0.65</sub> Pt <sub>0.35</sub>	2.3746	KCu <sub>4</sub> S <sub>3</sub>
1.3765	CoPt	2.4007	RbCu <sub>4</sub> S <sub>3</sub>
1.3969	Fe(NH <sub>4</sub> ) <sub>4</sub> SbCl <sub>12</sub>	2.8069	AgTi

## Organic

1.452 Cu[SC(NH<sub>2</sub>)<sub>2</sub>]<sub>3</sub>Cl

$\frac{4}{m} \frac{2}{m} \frac{2}{m}$

P4/mcc  $D_{4h}^2$  No. 124

Inorganic - 3  
Organic - 1

## Inorganic

1.7615	BaO <sub>2</sub> · 8H <sub>2</sub> O	1.7717	CaO <sub>2</sub> · 8H <sub>2</sub> O
1.7647	SrO <sub>2</sub> · 8H <sub>2</sub> O		

## Organic

2.3699 2(N<sub>3</sub>)<sub>2</sub>Pb · 11SC(NH<sub>2</sub>)<sub>2</sub>

$\frac{4}{m} \frac{2}{m} \frac{2}{m}$

P4/nbm  $D_{4h}^3$  No. 125

Inorganic - 3  
Organic - 0

## Inorganic

0.3783	Hg <sub>3</sub> Sb <sub>2</sub> I <sub>4</sub>	1.7369	BeI <sub>2</sub>
0.8964	Pb <sub>4</sub> Pt		

## Organic

.....

$\frac{4}{m} \frac{2}{m} \frac{2}{m}$

P4/nnc  $D_{4h}^4$  No. 126

Inorganic - 4  
Organic - 1

## Inorganic

0.7451	Ca <sub>10</sub> (Mg, Fe) <sub>2</sub> Al <sub>4</sub> Si <sub>9</sub> O <sub>34</sub> (OH) <sub>4</sub>	0.7632	Ca <sub>18</sub> Mg <sub>2</sub> H <sub>6</sub> Si <sub>17</sub> Al <sub>10</sub> O <sub>72</sub>
0.7569	Ca <sub>10</sub> Al <sub>4</sub> (Mg, Fe) <sub>2</sub> Si <sub>9</sub> O <sub>34</sub> (OH) <sub>4</sub>	1.4964	Ag[Co(NH <sub>3</sub> ) <sub>2</sub> (NO <sub>2</sub> ) <sub>4</sub> ]

## Organic

1.4637 (CH<sub>3</sub>)<sub>8</sub>Si<sub>8</sub>O<sub>8</sub>

$\frac{4}{m} \frac{2}{m} \frac{2}{m}$

P4/mbm  $D_{4h}^5$  No. 127

Inorganic - 45  
Organic - 3

## Inorganic

0.1712	Mo <sub>5</sub> O <sub>14</sub>	0.3203	Hg <sub>5</sub> Pd <sub>2</sub>
0.2986	In <sub>4</sub> Ti <sub>3</sub>	0.4033	Pt(NH <sub>3</sub> ) <sub>4</sub> Cl <sub>2</sub> · H <sub>2</sub> O
0.2997	Ga <sub>5</sub> V <sub>2</sub>	0.4224	Pd(NH <sub>3</sub> ) <sub>4</sub> Cl <sub>2</sub> · H <sub>2</sub> O
0.3003	Ga <sub>5</sub> V <sub>2</sub>	0.5056	Ga <sub>2</sub> Nb <sub>3</sub>
0.3120	K <sub>0.475</sub> W <sub>3</sub>	0.5162	Be <sub>2</sub> Nb <sub>3</sub>
0.3124	K <sub>0.50</sub> FeF <sub>3</sub>	0.5190	Al <sub>2</sub> Th <sub>3</sub>

P4/mbm  $D_{4h}^5$  No. 127 (continued)

## Inorganic (continued)

0.5231	$Ge_2Th_3$	0.5661	$B_4Lu$
0.5276	$B_2V_3$	0.5662	$B_4Y$
0.5304	$B_2Nb_3$	0.5666	$B_4Gd$
0.5308	$Si_2Th_3$	0.5668	$B_4Th$
0.5314	$B_2Ta_3$	0.5669	$B_4Dy$
0.5321	$Si_2U_3$	0.5673	$B_4Sm$
0.5419	$(M_3)B_2$	0.5677	$B_4Ce$
0.5419	$Pb_2Cl_2C\theta_3$	0.5678	$B_4Er$
0.5430	$B_4Gd$	0.5682	$B_4Nd$
0.5437	$(M_3)B_2$	0.5708	$B_4Tb$
0.5572	$Ce_3Si_2$	0.5736	$B_4Ho$
0.5605	$B_4Tb$	0.6180	$Ge_2Th_3$
0.5619	$B_4U$	0.7189	$K_3SiF_7$
0.5653	$B_4Er$	0.7270	$(NH_4)_2SiF_6 \cdot NH_4F$
0.5654	$B_4Y$	1.0862	$Pb_2Br_2C\theta_3$
0.5656	$B_4Ho$	1.0881	$Pb_2Cl_2C\theta_3$
0.5658	$B_4Dy$		

## Organic

0.542	$Pb_2Cl_2C\theta_3$	1.088	$Pb_2Cl_2C\theta_3$
1.086	$Pb_2Br_2C\theta_3$		

 $\frac{4}{m} \frac{2}{m} \frac{2}{m}$ P4/mnc  $D_{4h}^6$  No. 128Inorganic - 13  
Organic - 0

## Inorganic

0.7097	$Cu(NH_3)_4PtCl_4$	1.4565	$(NH_4)_3ScF_6$
0.7187	$Pt(NH_3)_4PtCl_4$	1.4843	$Na_5Al_3F_{14}$
1.3465	$K_5NaCl_2(S_2O_6)_2$	1.7556	$Ca_4KFSi_8O_{20} \cdot 8H_2O$
1.4268	$H_4SiW_{12}O_{40} \cdot 31H_2O$	2.3386	$Al_7Cu_2Fe$
1.4326	$H_5BW_{12}O_{40} \cdot 31H_2O$	2.3405	$Al_7CoCu_2$
1.4375	$(NH_4)_5BW_{12}O_{40} \cdot 26H_2O$	2.3469	$Al_7Cu_2Fe$
1.4528	$(NH_4)_3InF_6$		

## Organic

.....

 $\frac{4}{m} \frac{2}{m} \frac{2}{m}$ P4/nmm  $D_{4h}^7$  No. 129Inorganic - 160  
Organic - 39

## Inorganic

0.6657	$Na_4B_2O_4Cl_2 \cdot 4H_2O$	1.2650	$KUO_2AsO_4 \cdot 4H_2O$
0.6669	$NH_4SH$	1.2687	$SnO$
0.6717	$NH_4Br$	1.2714	$(K, Ba)(UO_2)(PO_4) \cdot 3H_2O$
0.7071	$NH_4I$	1.2882	$(UO_2)HPO_4 \cdot 4H_2O$
0.7098	$NH_4Br$	1.2940	$(Bi, Pb)_2O_3$
0.7099	$NH_4Br$	1.3687	$FeS$
0.7245	$PH_4Br$	1.3890	$YOF$
0.7393	$Li_xWO_3$	1.4268	$LaOF$
0.7422	$Na_{0.1}WO_3$	1.4433	$ThN_{0.9}F_{1.3}$
0.7457	$WO_3$	1.4656	$FeSe$
0.9532	$BiIn$	1.4673	$K_2NbOF_5$
0.9546	$BiIn$	1.5258	$Cu_2Sb$
1.0424	$Li_3UF_7$	1.5377	$Cu_{2.8}Te_2$
1.1918	$UO_2HASO_4 \cdot 4H_2O$	1.5430	$AgCuSe$
1.2070	$Ca(UO_2)_2(PO_4)_2 \cdot 6H_2O$	1.5748	$AsCuMg$
1.2070	$Ba(UO_2)_2(PO_4)_2 \cdot 8H_2O$	1.6029	$Ni_3Te_2$
1.2111	$Ca(UO_2)_2(PO_4)_2 \cdot 2-6H_2O$	1.6079	$Mn_2Sb$
1.2212	$LiOH$	1.6253	$BaHBr$
1.2219	$NaUO_2AsO_4 \cdot 4H_2O$	1.6294	$BaHI$
1.2222	$Cu(UO_2)_2(AsO_4)_2 \cdot 8H_2O$	1.6341	$BaHCl$
1.2248	$Ba(UO_2)_2(PO_4)_2 \cdot 6H_2O$	1.6442	$FeTe_{0.9}$
1.2253	$Ca(UO_2)_2(AsO_4)_2 \cdot 8H_2O$	1.6468	$AsFe_2$
1.2275	$NH_4(UO_2)(AsO_4) \cdot 3H_2O$	1.6613	$BiOF$
1.2291	$HUO_2AsO_4 \cdot 4H_2O$	1.6616	$BiOF$
1.2384	$Cu(UO_2)_2(AsO_4)_2 \cdot 8H_2O$	1.6659	$AcOCl$
1.2468	$Na(UO_2)(PO_4) \cdot 4H_2O$	1.6662	$AsMn_2$
1.2471	$Cu(UO_2)_2(PO_4)_2 \cdot 8H_2O$	1.6710	$LaOCl$
1.2637	$PbO$	1.6743	$CeOCl$

P4/nmm  $D_{4h}^7$  No. 129 (continued)

## Inorganic (continued)

1.6757	NdOCl	2.0022	SmOBr
1.6811	PrOCl	2.0040	Bi <sub>2</sub> U
1.6829	ThNCl	2.0140	LaTe <sub>2</sub>
1.6878	SmOCl	2.0161	PuOSe
1.6879	NdOCl	2.0192	PuS <sub>2-x</sub>
1.6885	EuOCl	2.0253	LaTe <sub>2</sub>
1.6891	GdOCl	2.0401	EuOBr
1.6902	YbCl	2.0426	EuOBr
1.6921	TbOCl	2.0461	Sb <sub>2</sub> U
1.6927	DyOCl	2.0482	Sb <sub>2</sub> U
1.6932	PuOCl	2.0505	CaHBr
1.6933	YbCl	2.0526	As <sub>2</sub> U
1.6950	AmOCl	2.0533	UNBr
1.6959	ErOCl	2.0536	As <sub>2</sub> U
1.6959	HoOCl	2.0628	BiOBr
1.6978	SrHCl	2.0699	NdTe <sub>1.8</sub>
1.7025	ThOS	2.0837	GdOBr
1.7128	UNCl	2.0888	BB <sub>4</sub>
1.7135	SrHBr	2.0986	As <sub>2</sub> Th
1.7145	U(NH)Cl	2.1071	Sb <sub>2</sub> Th
1.7331	CeSF	2.1123	TbOBr
1.7336	AcOBr	2.1254	DyOBr
1.7382	ThOSe	2.1302	NaHC <sub>2</sub>
1.7388	LaSF	2.1473	YbBr
1.7390	EuSF	2.1505	HoOBr
1.7396	NpOS	2.1627	ErOBr
1.7419	UOS	2.1776	ImOBr
1.7495	PaOS	2.1954	YbOBr
1.7518	AsCr <sub>1.74</sub> Fe <sub>0.26</sub>	2.1963	CaHI
1.7528	AsCr <sub>2</sub>	2.2026	LaOI
1.7628	PbFCl	2.2115	ZrGeS
1.7647	AsCr <sub>2</sub>	2.2121	YbOBr
1.7754	LaOBr	2.2243	ZrGeTe
1.7775	ZrS	2.2247	LuOBr
1.7816	CaHCl	2.2318	ZrGeSe
1.7888	UOSe	2.2684	PuOI
1.7918	AlNaSi <sub>4</sub>	2.2729	ZrSiS
1.8093	CeOBr	2.2912	BiOI
1.8158	PbFBr	2.2934	SmOI
1.8332	ThOTe	2.3083	UNI
1.8391	PrOBr	2.3089	ZrSiSe
1.8709	UOTe	2.3581	ImOI
1.8747	RbHC <sub>2</sub>	2.3672	YbOI
1.8824	PuOBr	2.4282	Ba(UO <sub>2</sub> ) <sub>2</sub> (PO <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> O
1.8879	NdOBr	2.4444	Cu(UO <sub>2</sub> ) <sub>2</sub> (AsO <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> O
1.8921	BiOCl	2.4719	Pb(UO <sub>2</sub> ) <sub>2</sub> (PO <sub>4</sub> ) <sub>2</sub> •8H <sub>2</sub> O
1.8941	CuTi	2.5729	ZrSiTe
1.8967	NdOBr	3.0833	CdTi
1.9040	AgZr	3.5858	(Ca, F)(BiO)CO <sub>3</sub>
1.9221	BiO(OH, Cl)	4.4569	Cu <sub>3</sub> Ti <sub>2</sub>
1.9332	SrHI	5.2210	Bi <sub>2</sub> SrO <sub>3</sub> Br <sub>2</sub>
1.9629	KHC <sub>2</sub>	5.3001	CaBi <sub>2</sub> O <sub>3</sub> Br <sub>2</sub>

## Organic

0.3884	[(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NCS <sub>2</sub> ] <sub>2</sub> Ni	1.9629	KHC <sub>2</sub>
0.708	(CH <sub>3</sub> ) <sub>4</sub> NMnO <sub>4</sub>	2.075	CH <sub>3</sub> HgCl
0.711	N(CH <sub>3</sub> ) <sub>4</sub> Cl	2.130	NaHC <sub>2</sub>
0.713	N(CH <sub>3</sub> ) <sub>4</sub> Br	2.1641	LiOCH <sub>3</sub>
0.7170	(CH <sub>3</sub> ) <sub>4</sub> NClO <sub>4</sub>	2.167	C <sub>2</sub> H <sub>5</sub> HgBr
0.7240	N(CH <sub>3</sub> ) <sub>4</sub> I	2.220	CH <sub>3</sub> KO
0.836	CH <sub>3</sub> NH <sub>3</sub> Cl	2.327	C <sub>2</sub> H <sub>5</sub> HgCl
0.8452	(CH <sub>3</sub> ) <sub>3</sub> P•BH <sub>3</sub>	2.559	Na(CH <sub>3</sub> ) <sub>2</sub> / <sub>3</sub> (OH) <sub>1/3</sub>
0.8672	C <sub>4</sub> H <sub>9</sub> Cl	2.6118	BiO•O•O•CH
1.0579	C <sub>3</sub> H <sub>7</sub> NH <sub>3</sub> I	2.6621	C <sub>24</sub> H <sub>18</sub>
1.136	C <sub>3</sub> H <sub>7</sub> NH <sub>3</sub> Br	2.8551	C <sub>6</sub> H <sub>5</sub> HgI
1.186	C <sub>3</sub> H <sub>7</sub> NH <sub>3</sub> Cl	2.898	C <sub>3</sub> H <sub>7</sub> HgCl
1.711	NaOCH <sub>3</sub>	3.0084	C <sub>6</sub> H <sub>5</sub> HgCl
1.719	NH <sub>3</sub> CH <sub>3</sub> Br	3.1940	CH <sub>3</sub> COO•O•Bi
1.751	NH <sub>3</sub> CH <sub>3</sub> I	3.5858	(Ca, F)(BiO)CO <sub>3</sub>
1.8747	RbHC <sub>2</sub>	3.8355	BiO•O•O•CC <sub>2</sub> H <sub>5</sub>

P4/nmm  $D_{4h}^7$  No. 129 (continued)

## Organic (continued)

4.252	$C_7H_{15}NH_3Cl$	5.423	$C_{10}H_{21}NH_3I$
4.4615	$Bi\theta\theta\theta CC_3H_7$	5.880	$C_{11}H_{23}NH_3I$
4.575	$C_8H_{17}NH_3I$	6.031	$C_{12}H_{25}NH_3I$
5.128	$Bi\theta\theta\theta CC_4H_9$		

$\frac{4}{m} \frac{2}{m} \frac{2}{m}$

P4/ncc  $D_{4h}^8$  No. 130

Inorganic - 26  
Organic - 2

## Inorganic

0.6842	$CuBi_4\theta_7$	2.4596	$(Rb, H_3\theta)(U\theta_2)(As\theta_4)\theta_3H_2\theta$
1.2867	$Sr(\theta H)_2\theta_8H_2\theta$	2.4615	$H_3\theta(U\theta_2)(As\theta_4)\theta_3H_2\theta$
1.5460	$Sr_3Si\theta_5$	2.4848	$(Na, H_3\theta)(U\theta_2)(P\theta_4)\theta_3H_2\theta$
1.9600	$Ba_5Si_3$	2.4914	$(K, H_3\theta)(U\theta_2)(As\theta_4)\theta_3H_2\theta$
2.0712	$CaCuSi_4\theta_{10}$	2.5025	$H_3\theta(U\theta_2)(P\theta_4)\theta_3H_2\theta$
2.1126	$CuSrSi_4\theta_{10}$	2.5168	$K(H_3\theta)(U\theta_2As\theta_4)_2\theta_6H_2\theta$
2.1414	$BaFeSi_4\theta_{10}$	2.5259	$K(U\theta_2)As\theta_4\theta_3H_2\theta$
2.1578	$BaMgSi_4\theta_{10}$	2.5308	$NH_4(U\theta_2)(As\theta_4)\theta_3H_2\theta$
2.1653	$BaCuSi_4\theta_{10}$	2.5434	$(K, H_3\theta)(U\theta_2)(P\theta_4)\theta_3H_2\theta$
2.3961	$Ag(U\theta_2)(As\theta_4)\theta_3H_2\theta$	2.5629	$(Rb, H_3\theta)(U\theta_2)(P\theta_4)\theta_3H_2\theta$
2.4376	$Ag(U\theta_2)(P\theta_4)\theta_3H_2\theta$	2.5766	$(NH_4)(U\theta_2)(P\theta_4)\theta_3H_2\theta$
2.4472	$(H_3\theta, Na)(U\theta_2)(As\theta_4)\theta_3H_2\theta$	2.6290	$(H_3\theta, Li)(U\theta_2)(P\theta_4)\theta_3H_2\theta$
2.4566	$(H_3\theta, Li)(U\theta_2)(As\theta_4)\theta_3H_2\theta$	3.0549	$Mo_6Cl_8(Cl_4\theta_2H_2\theta)\theta_6H_2\theta$

## Organic

1.0236	$Pt(C_2H_5NH_2)_4\theta Pt(C_2H_5NH_2)_4Br_2\theta Br_4$	1.3763	$(CH_3)_4N\theta I\theta_4$
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$\frac{4}{m} \frac{2}{m} \frac{2}{m}$

P4<sub>2</sub>/mmc  $D_{4h}^9$  No. 131

Inorganic - 7  
Organic - 1

## Inorganic

0.8599	$SrPbF_6$	1.7566	Pt $\theta$
1.2754	$C_2Th$	1.7579	PtS
1.2770	$C_2Th$	1.7607	PtS
1.7546	Pd $\theta$		

## Organic

1.275	ThC <sub>2</sub>
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$\frac{4}{m} \frac{2}{m} \frac{2}{m}$

P4<sub>2</sub>/mcm  $D_{4h}^{10}$  No. 132

Inorganic - 2  
Organic - 1

## Inorganic

1.4660	$AgUF_6$	1.8269	$NH_4CN$
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## Organic

1.827	$NH_4CN$
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$\frac{4}{m} \frac{2}{m} \frac{2}{m}$

P4<sub>2</sub>/nbc  $D_{4h}^{11}$  No. 133

Inorganic - 2  
Organic - 0

## Inorganic

0.4971	$V_3S$	1.4785	$(Mn, Ca, Zn)Te_2\theta_5$
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## Organic

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$\frac{4}{m} \frac{2}{m} \frac{2}{m}$

P4<sub>2</sub>/nmm  $D_{4h}^{12}$  No. 134

Inorganic - 6  
Organic - 1

## Inorganic

0.5651	$B_{25}Ni$	0.8112	AlB <sub>12</sub>
0.5801	B	1.0682	$CuSn(\theta H)_6$
0.8110	$Al_3B_{44}C_2$	1.4565	$NH_4As(Mo\theta_4)_3\theta_2H_2\theta$

$P4_2/nmm$   $D_{4h}^{12}$  No. 134 (continued)

Organic  
0.8110  $Al_3B_{44}C_2$

$\frac{4}{m} \frac{2}{m} \frac{2}{m}$

$P4_2/mbc$   $D_{4h}^{13}$  No. 135

Inorganic - 11  
Organic - 0

Inorganic

0.6047	$Se\theta_2$	0.6961	$CoSb_2\theta_4$
0.6473	$CuAs_2\theta_4$	0.6972	$ZnSb_2\theta_4$
0.6837	$NIAs_2\theta_4$	0.6995	$MgSb_2\theta_4$
0.6873	$FeSb_2\theta_4$	0.7078	$NI Sb_2\theta_4$
0.6885	$MnSb_2\theta_4$	0.7225	$Pb_2Sn\theta_4$
0.6892	$FeSb_2\theta_4$		

Organic

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$\frac{4}{m} \frac{2}{m} \frac{2}{m}$

$P4_2/mmm$   $D_{4h}^{14}$  No. 136

Inorganic - 112  
Organic - 4

Inorganic

0.3643	$Nb\theta Cl_3$	0.6527	$GaTa\theta_4$
0.5115	$MnTi$	0.6547	$TiTa\theta_4$
0.5138	$NaK(Ca, Mg, Mn)Al_4Si_5\theta_{18} \cdot 8H_2\theta$	0.6559	$Fe\theta F$
0.5164	$Cr_7Fe_8$	0.6565	$AlSb\theta_4$
0.5176	$Co_{13}Cr_{17}$	0.6595	$MgF_2$
0.5176	$Ni_2V_3$	0.6599	$Cr\theta_2$
0.5177	$Cr_2Ru$	0.6601	$GaSb\theta_4$
0.5189	$CoCr$	0.6601	$MgF_2$
0.5192	$MoRe$	0.6620	$NiF_2$
0.5209	$ReW$	0.6620	$(Sn, Fe)(\theta, \theta H)_2$
0.5216	$AlNb_2$	0.6631	$NiF_2$
0.5221	$FeMo$	0.6646	$CrSb\theta_4$
0.5230	$Co_2Mo_3$	0.6653	$ZnF_2$
0.5237	$(Fe, Mo)$	0.6662	$ZnF_2$
0.5324	$AlTa_2$	0.6681	$SbV\theta_4$
0.5700	$W\theta_2$	0.6687	$MgH_2$
0.5741	$Mo\theta_2$	0.6690	$MgD_2$
0.5768	$Be\theta$	0.6694	$SbV\theta_4$
0.6136	$Ni_2$	0.6710	$(Sn, Fe, Ti, Ta, Nb)\theta_2$
0.6203	$Nb\theta_2$	0.6724	$Sn\theta_2$
0.6344	$V\theta_2$	0.6738	$RhSb\theta_4$
0.6345	$RhV\theta_4$	0.6772	$CoF_2$
0.6358	$TiNb\theta_4$	0.6792	$MnF_2$
0.6377	$Si\theta_2$	0.6797	$MnF_2$
0.6387	$Fe(Nb, Ta)_2\theta_6 \cdot 5Ti\theta_2$	0.6801	$CoF_2$
0.6396	$RhV\theta_4$	0.6827	$Pb\theta_2$
0.6423	$RhNb\theta_4$	0.6838	$PdF_2$
0.6432	$RhNb\theta_4$	0.6896	$Ru\theta_2$
0.6438	$Ti\theta_2$	0.6918	$Ru\theta_2$
0.6441	$TiV\theta_4$	0.6957	$FeF_2$
0.6443	$Ti\theta_2$	0.6993	$Ir\theta_2$
0.6447	$RhTa\theta_4$	0.7046	$FeF_2$
0.6452	$CoNb_2\theta_6$	0.7073	$\theta_2$
0.6464	$NiNb_2\theta_6$	0.7871	$Te\theta_2$
0.6479	$VNb\theta_4$	0.8882	$Li_2Sr_3$
0.6481	$CrNb\theta_4$	0.9123	$Zn_2Zr_3$
0.6481	$FeNb\theta_4$	0.9165	$Al_2Hf_3$
0.6489	$AlTa\theta_4$	0.9172	$Al_2Zr_3$
0.6489	$(Fe, Mn)(Ta, Nb)_2\theta_6$	0.9268	$Al_2Y_3$
0.6503	$CrTa\theta_4$	1.0000	$(NH_4)_2CuBr_4 \cdot 2NH_3$
0.6507	$Ge\theta_2$	1.0243	$Rb_2CuCl_4 \cdot 2H_2\theta$
0.6507	$Mn\theta_2$	1.0407	$Ca_2CuCl_4 \cdot 2H_2\theta$
0.6508	$VTa\theta_4$	1.0484	$(NH_4)_2CuCl_4 \cdot 2H_2\theta$
0.6509	$Ta\theta_2$	1.0539	$(NH_4)_2CuBr_4 \cdot 2H_2\theta$
0.6511	$FeTa\theta_4$	1.0577	$K_2CuCl_4 \cdot 2H_2\theta$
0.6513	$FeSb\theta_4$	1.0976	$(NH_4)_2MnCl_4 \cdot 2H_2\theta$
0.6515	$FeTa\theta_4$	1.8129	$Pt(NH_3)_2Cl_4$
0.6516	$FeNb\theta_4$	1.9362	$NiTa_2\theta_6$
0.6521	$Mn\theta_2$	1.9366	$CoTa_2\theta_6$

P4<sub>2</sub>/mmm D<sub>4h</sub><sup>14</sup> No. 136 (continued)

## Inorganic (continued)

1.9410	(Fe,Mn)(Ta,Nb) <sub>2</sub> O <sub>6</sub>	1.9785	Zn(SbO <sub>3</sub> ) <sub>2</sub>
1.9532	MgTa <sub>2</sub> O <sub>6</sub>	1.9827	NiSb <sub>2</sub> O <sub>6</sub>
1.9572	Al <sub>2</sub> TeO <sub>6</sub>	1.9828	ZnSb <sub>2</sub> O <sub>6</sub>
1.9572	FeTa <sub>2</sub> O <sub>6</sub>	1.9880	Fe <sub>2</sub> TeO <sub>6</sub>
1.9679	Mg(SbO <sub>3</sub> ) <sub>2</sub>	1.9892	FeSb <sub>2</sub> O <sub>6</sub>
1.9758	Ga <sub>2</sub> TeO <sub>6</sub>	1.9892	MgSb <sub>2</sub> O <sub>6</sub>
1.9780	Cr <sub>2</sub> TeO <sub>6</sub>	1.9935	CoSb <sub>2</sub> O <sub>6</sub>

## Organic

1.1938	C <sub>16</sub> H <sub>16</sub>	1.2712	C <sub>4</sub> H <sub>6</sub>
1.2536	C <sub>6</sub> H <sub>10</sub> Cl <sub>2</sub>	2.1246	P <sub>2</sub> Cl <sub>2</sub> S <sub>2</sub> N <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub>

4 2 2  
m m m

P4<sub>2</sub>/nmc D<sub>4h</sub><sup>15</sup> No. 137

Inorganic - 12  
Organic - 4

## Inorganic

0.6737	B <sub>4</sub> Cl <sub>4</sub>	2.7174	ZnI <sub>2</sub>
0.9234	H <sub>2</sub> O	2.8200	HgI <sub>2</sub>
1.4041	Cd <sub>3</sub> P <sub>2</sub>	2.8368	HgI <sub>2</sub>
1.4141	P <sub>2</sub> Zn <sub>3</sub>	2.8548	HgI <sub>2</sub>
1.4142	As <sub>2</sub> Cd <sub>3</sub>	2.8555	Cu <sub>2</sub> HgI <sub>4</sub>
1.4478	ZrO <sub>2</sub>	2.8649	ZnCl <sub>2</sub>

## Organic

0.5417	LiAl(C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub>	0.7424	(HgOSi(CH <sub>3</sub> ) <sub>4</sub> ) <sub>2</sub>
0.6334	(PCF <sub>3</sub> ) <sub>4</sub>	1.6586	[(C <sub>2</sub> H <sub>5</sub> ) <sub>4</sub> N] <sub>2</sub> NiCl <sub>4</sub>

4 2 2  
m m m

P4<sub>2</sub>/nmc D<sub>4h</sub><sup>16</sup> No. 138

Inorganic - 3  
Organic - 0

## Inorganic

0.7150	Cl <sub>2</sub>	3.1563	AuI
1.2285	NH <sub>4</sub> NO <sub>3</sub>		

## Organic

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4 2 2  
m m m

I4/mmm D<sub>4h</sub><sup>17</sup> No. 139

Inorganic - 215  
Organic - 24

## Inorganic

0.1897	WV <sub>2</sub> O <sub>8-x</sub>	0.5871	Be <sub>12</sub> Co
0.3618	V <sub>4</sub> Zn <sub>5</sub>	0.7101	Be <sub>3</sub> Ca <sub>8</sub> AlSi <sub>8</sub> O <sub>28</sub> (OH)•4H <sub>2</sub> O
0.3779	(Cu,Tl,Ag) <sub>2</sub> Se	0.9406	AgBrO <sub>3</sub>
0.4693	Pt <sub>3</sub> Tl	0.9585	Mo <sub>0.2</sub> U <sub>0.8</sub>
0.5368	Cu(NH <sub>3</sub> ) <sub>4</sub> (CuCl <sub>2</sub> ) <sub>2</sub> •H <sub>2</sub> O	1.0000	TiCl <sub>4</sub> •4NH <sub>3</sub>
0.5410	HgTlS <sub>2</sub>	1.0089	Ta <sub>2</sub> H
0.5514	Cu(NH <sub>3</sub> ) <sub>4</sub> (CuBr <sub>2</sub> ) <sub>2</sub>	1.0549	FeN <sub>x</sub>
0.5664	Mn <sub>12</sub> Th	1.0724	[(NH <sub>3</sub> ) <sub>4</sub> Cl <sub>2</sub> Pt]Cl <sub>2</sub>
0.5727	Be <sub>12</sub> W	1.0996	Fe <sub>8</sub> N
0.5734	Al <sub>3</sub> CeFe <sub>4</sub>	1.1366	K <sub>3</sub> TlCl <sub>6</sub> •2H <sub>2</sub> O
0.5752	Mg <sub>12</sub> Nd	1.1475	Rb <sub>3</sub> TlBr <sub>6</sub> •1.14 <sub>3</sub> H <sub>2</sub> O
0.5772	Be <sub>12</sub> Cr	1.1798	V <sub>2</sub> O <sub>5</sub> •532
0.5773	Be <sub>12</sub> Nb	1.2519	K <sub>2</sub> Sb <sub>2</sub> Cl <sub>4</sub>
0.5783	Mg <sub>12</sub> Pr	1.3211	Mn
0.5787	Be <sub>12</sub> V	1.3315	Pu
0.5818	Be <sub>12</sub> Ta	1.3467	Ni
0.5823	Be <sub>12</sub> Mo	1.3766	Cd <sub>0.6</sub> Zr <sub>0.4</sub>
0.5835	Be <sub>12</sub> Fe	1.4194	Cs <sub>3</sub> YF <sub>6</sub>
0.5845	YZn <sub>12</sub>	1.4197	Cs <sub>3</sub> TlF <sub>6</sub>
0.5848	Al <sub>3</sub> CeCu <sub>4</sub>	1.4347	Rb <sub>3</sub> TlF <sub>6</sub>
0.5849	Be <sub>12</sub> Mn	1.4351	Rb <sub>3</sub> YF <sub>6</sub>
0.5861	HoZn <sub>12</sub>	1.4513	Cs <sub>2</sub> AuAuCl <sub>6</sub>

14/mmm  $D_{4h}^{17}$  No. 139 (continued)

## Inorganic (continued)

1.4677	$K_3YF_6$	2.5063	$Ni_2Ta$
1.4919	$Cs_2AgAuCl_6$	2.5233	$Pd_2Zr$
1.5203	In	2.5287	$Al_{2.8}Be_{1.2}Ce$
1.5607	Ga	2.5550	$Au_2Mn$
1.6045	$BaC_2$	2.5929	$Al_2CeZn_2$
1.6071	Tl	2.6342	$Al_2CeGa_2$
1.6199	$XeF_2$	2.6350	$Cr_2Ge_2Th$
1.6208	$Cu_4Pb_4Cl_8O_4 \cdot 5H_2O$	2.6770	$Ge_2Mn_2Th$
1.6253	$C_2Sr$	2.7730	$Al(UO_2)_4R(PO_4)_4 \cdot 16H_2O$
1.6309	$C_2Nd$	2.8078	$Mg(UO_2)_2(AsO_4)_2 \cdot 9 \cdot 10H_2O$
1.6374	$CsO_2$	2.8385	$Mg(UO_2)_2[(P_{1-x}As_x)O_4]_2 \cdot 10H_2O$
1.6401	$C_2Ca$	2.8696	$MoU_2$
1.6557	$C_2La$	2.8790	$Cu(UO_2)_2(AsO_4)_2 \cdot 10H_2O$
1.6580	$RbO_2$	2.9078	$Cu(UO_2)_2(PO_4)_2 \cdot 8H_2O$
1.6610	$KO_2$	2.9518	$Ca(UO_2)_2(PO_4)_2 \cdot 10.5H_2O$
1.6675	$KO_2$	2.9574	$Cu(UO_2)_2(PO_4)_2 \cdot 12H_2O$
1.6679	$C_2Pr$	2.9781	HgF
1.6706	$C_2La$	2.9789	$Ca(UO_2)_2(PO_4)_2 \cdot 10-12H_2O$
1.6714	$C_2Ce$	3.0219	$K_2UO_4$
1.6723	$CaO_2$	3.0662	$K_2CuF_4$
1.6727	$C_2Nd$	3.0832	$Ba_2PbO_4$
1.7023	$C_2U$	3.0959	$Ba_2PbO_4$
1.7042	$C_2U$	3.1038	$Sr_2SnO_4$
1.7910	$BaO_2$	3.1287	$Bi_3NaO_4Cl_2$
1.7974	$BaO_2$	3.1328	$(LiBi_3)O_4Cl_2$
1.8451	$SrO_2$	3.1336	$Rb_2CuF_4$
1.8907	$PbF_4$	3.1352	$K_2FeF_4$
1.9590	$SnF_4$	3.1541	$PbSbO_2Cl$
1.9774	$Na_3HfF_7$	3.1830	$Rb_2UO_4$
1.9774	$Na_3ZrF_7$	3.1974	$Bi_3NaO_4Br_2$
1.9847	$Na_3PaF_8$	3.2078	$Bi_2O_{3-x}$
1.9926	$Na_3TbF_7$	3.2091	$Cs_2CdCl_4$
1.9932	$3Mn_2O_3 \cdot MnSiO_3$	3.2106	$K_2CoF_4$
1.9988	$NbF_4$	3.2114	$Ba_2SnO_4$
2.0000	$NbF_4$	3.2131	$Ba_2SnO_4$
2.0000	$Na_3UF_7$	3.2172	$Bi_3LiO_4Br_2$
2.0000	$Na_3UF_8$	3.2297	$BaBiO_2Cl$
2.0153	$Pd_3V$	3.2359	$Rb_2ZnF_4$
2.0264	$Pt_3V$	3.2441	$Sr_2TiO_4$
2.0362	$Ni_3V$	3.2448	$BaBiO_2Br$
2.2264	$Al_3Ta$	3.2474	$Sr_2TiO_4$
2.2364	$Al_3Ti$	3.2487	$K_2ZnF_4$
2.2372	$Al_3Nb$	3.2532	$Tl_2CuF_4$
2.2673	$Al_3Hf$	3.2641	$K_2NiF_4$
2.3091	$In_3Zr$	3.2755	$Sr_2MoO_4$
2.3105	$Al_4Sm$	3.2797	$Sr_2MnO_4$
2.3164	$Au_2Zr$	3.2820	$La_2NiO_4$
2.3256	$Ge_2Ni_2Th$	3.2916	$Ca_2MnO_4$
2.3259	$Al_4La$	3.3059	$Rb_2CoF_4$
2.3598	$Hg_2I_2$	3.3062	$K_2MgF_4$
2.3618	$BaGa_4$	3.3213	$Sr_2IrO_4$
2.3871	$Hg_2Br_2$	3.3248	$Pb_4O_4Cl_2$
2.3873	$K_4(Ru_2Cl_{10}O) \cdot H_2O$	3.3333	$LaSrAlO_4$
2.4176	$Co_2Ge_2Th$	3.3350	$CdBiO_2I$
2.4212	$Ga_4Sr$	3.3358	$Bi_3NaO_4I_2$
2.4220	$Ga_4Yb$	3.3465	$PdZr_2$
2.4233	$NbP_{0.95}$	3.3469	$Bi_3LiO_4I_2$
2.4233	$P_{0.95}Ta$	3.3545	$Rb_2NiF_4$
2.4253	$EuGa_4$	3.3766	$(NH_4)_2NiF_4$
2.4413	$ThZn_4$	3.3767	$Cs_2UO_4$
2.4422	$Cu_2Ge_2Th$	3.3802	$Sr_2FeO_3F$
2.4472	$Hg_2Cl_2$	3.4242	$CuZr_2$
2.4522	$MoSi_2$	3.4390	$Tl_2CoF_4$
2.4533	$Si_2W$	3.4555	$K_2NbO_3F$
2.4566	$MoSi_2$	3.5102	$Tl_2NiF_4$
2.4592	$Al_4Ba$	3.5393	$Bi_2O_2CO_3$
2.4736	$Ge_2Mo$	3.6640	$CuTi_2$
2.4747	$CaGa_4$	3.8617	$Bi_2Pd$
2.4831	$Al_4Sr$	3.9476	$RhSn_2$
2.4898	$Au_2Ti$	3.9908	$Pb_9Cu_8Ag_3Cl_{21}(OH)_{16} \cdot H_2O$
2.4944	$Fe_2Ge_2Th$	4.0000	$AgTi_2$
2.5041	$Ag_2Y$	4.2951	$Bi_2TiO_4F_2$
2.5059	$Al_3CeCu$	4.3006	$Al_3Hf$
2.5062	$K_4Re_2O_{10} \cdot H_2O$	4.3159	$Al_3Zr$

I4/mmm  $D_{4h}^{17}$  No. 139 (continued)

## Inorganic (continued)

4.3364	$Bi_2Nb_5F$	7.2051	$Sr_4Ti_3\sigma_{10}$
4.3458	$Bi_2Ta_5F$	7.2072	$Ca_4Mn_3\sigma_{10}$
4.6841	$CdTi_2$	7.2379	$Bi_3Sr_4Br_3$
5.1210	$K_3Fe_2F_7$	7.9033	$Bi_3Sr_4I_3$
5.2227	$K_8Zn_2F_7$	8.5473	$Bi_4Ti_3\sigma_{12}$
5.2256	$Sr_3Ti_2\sigma_7$	8.8571	$Bi_3\sigma_4$
5.4541	$Bi_{1.5}Cd_{1.25}\sigma_2Cl_3$	9.3154	$Bi_3+2x Cd_{2-3x}\sigma_4Cl_5$
5.5658	$Bi_{1.5}Ca_{1.25}\sigma_2Cl_3$	9.3546	$Bi_3+2x Ca_{2-3x}\sigma_4Cl_5$
5.7194	$Bi_{1.65}Cd_{1.03}\sigma_2Br_3$	9.9079	$Bi_3+2x Cd_{2-3x}\sigma_4Br_5$
5.7579	$CaBi_2\sigma_2(C\sigma_3)_2$	10.8705	$BaBi_4Ti_4\sigma_{15}$
6.3706	$Cu_4Ti_3$	13.0815	$Bi_5+2x Cd_{2-3x}\sigma_6Cl_7$
6.8532	$Bi_3Sr_4Cl_3$		

## Organic

0.6486	$(C_5H_5NH)HReBr_4$	1.7023	$UC_2$
0.9743	$C(SCH_3)_4$	1.7042	$UC_2$
1.1018	$C_2(CH_3)_4Br_2$	2.809	$Tl(CH_3)_2I$
1.605	$BaC_2$	3.083	$Tl(CH_3)_2Br$
1.625	$SrC_2$	3.094	$C_8\sigma C_8\sigma C_8\sigma$
1.631	$NdC_2$	3.157	$Rb\sigma C_8\sigma C_8\sigma Rb$
1.6401	$CaC_2$	3.247	$K\sigma C_8\sigma C_8\sigma K$
1.6557	$LaC_2$	3.267	$Tl(CH_3)_2Cl$
1.6679	$PrC_2$	3.3396	$(CH_3)_2SnF_2$
1.6706	$LaC_2$	3.4126	$Na\sigma C_8\sigma C_8\sigma Na$
1.6714	$CeC_2$	3.539	$Bi_2\sigma_2C\sigma_3$
1.6727	$NdC_2$	5.7579	$CaBi_2\sigma_2(C\sigma_3)_2$

 $\frac{4}{m} \frac{2}{m} \frac{2}{m}$ I4/mcm  $D_{4h}^{18}$  No. 140Inorganic - 99  
Organic - 3

## Inorganic

0.4921	$BFe_{4.7}Si_2$	0.8462	$InTe$
0.4926	$BCo_{4.7}Si_2$	0.8509	$BNi_2$
0.5000	$Ga_3Ta_5$	0.8519	$BW_2$
0.5012	$Ga_3Ta_5$	0.8542	$BMo_2$
0.5024	$NiU_6$	0.8595	$CoZr_2$
0.5029	$CoU_6$	0.8596	$Sb_2V$
0.5030	$SbTi_3$	0.8726	$Sb_2Ti$
0.5056	$Cr_5Si_3$	0.8728	$TlSe$
0.5078	$Cr_5Ge_3$	0.8729	$TlS$
0.5082	$FeU_6$	0.8811	$CoSc_2$
0.5092	$MnU_6$	0.8820	$RhSn_2$
0.5094	$Mo_5Si_3$	1.1537	$KSCN$
0.5141	$FePu_6$	1.1561	$KCN\sigma$
0.5153	$Si_3W_5$	1.1579	$KN_3$
0.6157	$US_2$	1.1651	$RbN_3$
0.7445	$AuNa_2$	1.2010	$KHF_2$
0.7710	$AuPb_2$	1.2305	$RbHF_2$
0.7716	$AlTh_2$	1.2318	$CsN_3$
0.7725	$AgTh_2$	1.2769	$CsHF_2$
0.7850	$InTh_2$	1.3411	$KCuF_3$
0.7885	$CuTh_2$	1.4425	$SiU_3$
0.7928	$AlHf_2$	1.5232	$Ir_3Si$
0.8007	$SiZr_2$	1.5358	$Ba_3Si\sigma_5$
0.8019	$AuTh_2$	1.5513	$Ga_5Pd$
0.8025	$AlZr_2$	1.5763	$Ba_2LaAl\sigma_5$
0.8060	$Al_2Cu$	1.5777	$Ba_3Ge\sigma_5$
0.8090	$PdTh_2$	1.5787	$Cs_3CoCl_5$
0.8092	$NiZr_2$	1.5842	$Ba_3V\sigma_5$
0.8122	$FeSn_2$	1.5937	$Ba_3Co\sigma_5$
0.8155	$GeHf_2$	1.5943	$Ba_3Cr\sigma_5$
0.8158	$AgIn_2$	1.5981	$Ba_2SrCo\sigma_5$
0.8162	$SiZr_2$	1.6042	$Sr_2LaAl\sigma_5$
0.8174	$BMn_2$	1.6048	$Ba_3Fe\sigma_5$
0.8175	$MnSn_2$	1.6118	$Ba_3Ti\sigma_5$
0.8184	$SiTa_2$	1.6125	$Ba_2LaGa\sigma_5$
0.8235	$K\sigma_3$	1.6148	$Ba_2LaFe\sigma_5$
0.8315	$BFe_2$	1.6159	$Ba_3V\sigma_5$
0.8324	$BCr_2$	1.6230	$Sr_2LaGa\sigma_5$
0.8386	$FeGe_2$	1.6236	$Ba_2LaCo\sigma_5$
0.8414	$BCo_2$	1.6400	$Ba_3Mn\sigma_5$



I4/mcm  $D_{4h}^{18}$  No. 140 (continued)

## Inorganic (continued)

1.7092	$NH_4Pb_2Br_5$	1.8628	$B_2Fe_5Si$
1.7136	$Pb_3(CoCl_4)Cl$	1.8636	$Ba_5Pb_3$
1.7241	$RbPb_2Br_5$	1.8671	$Ag_3Ca_5$
1.7322	$KPb_2Br_5$	1.8819	$B_2Co_5P$
1.7983	$KBrF_4$	1.8847	$B_2Fe_5P$
1.8079	$Nb_5Si_3$	1.8935	$B_2Mn_5P$
1.8085	$Ga_3Te_5$	1.9487	$B_3Cr_5$
1.8200	$Ge_3Te_5$	1.9487	$B_2Mo_5Si$
1.8221	$Si_3Te_5$	4.5269	$Au_{75}Ga_7Zn_{18}$
1.8610	$B_2Mn_5Si$		

## Organic

0.7408	$Co(C_5H_5)_2 \cdot Cl_4$	1.1561	$KCN_6$
1.1537	$KSCN$		

$\frac{4}{m} \frac{2}{m} \frac{2}{m}$

I4<sub>1</sub>/amd  $D_{4h}^{19}$  No. 141

Inorganic - 155  
Organic - 7

## Inorganic

0.4964	$Ca_3V_8O_{22} \cdot 15H_2O$	0.8865	$ThBr_4$
0.5361	$InSb$	0.8876	$(Th, U)Si_4O_4$
0.5380	$AlSb$	0.8880	$GdAs_4O_4$
0.5455	$Sn$	0.8889	$SmAs_4O_4$
0.5492	$GaSb$	0.8890	$(Th, U)Si_4O_4$
0.6400	$YbZn_{11}$	0.8896	$PaSi_4O_4$
0.6412	$Cd_{11}Eu$	0.8907	$DyAs_4O_4$
0.6439	$BaCd_{11}$	0.8917	$Th_3(V_6O_4)_4$
0.6948	$TeI_4$	0.8924	$YAs_4O_4$
0.8623	$CaCr_4O_4$	0.8927	$YbAs_4O_4$
0.8671	$YVO_4$	0.8932	$PaCl_4$
0.8688	$YPO_4$	0.8939	$EuAs_4O_4$
0.8735	$YPO_4$	0.8943	$ErAs_4O_4$
0.8745	$CaCr_4O_4$	0.8946	$TbAs_4O_4$
0.8752	$(Y, Er)PO_4$	0.8950	$TmAs_4O_4$
0.8753	$ErPO_4$	0.8953	$USi_4O_4$
0.8753	$PrCr_4O_4$	0.8953	$HoAs_4O_4$
0.8757	$NdCr_4O_4$	0.8955	$USi_4O_4$
0.8764	$EuCr_4O_4$	0.8983	$NpSi_4O_4$
0.8766	$GdCr_4O_4$	0.8997	$YPO_4$
0.8766	$SmCr_4O_4$	0.9008	$PuSi_4O_4$
0.8771	$NdVO_4$	0.9012	$ZrSi_4O_4$
0.8778	$TbCr_4O_4$	0.9021	$ThGe_4O_4$
0.8783	$DyCr_4O_4$	0.9021	$UCl_4$
0.8783	$CeVO_4$	0.9025	$AmSi_4O_4$
0.8785	$HoCr_4O_4$	0.9027	$ScVO_4$
0.8785	$SmVO_4$	0.9045	$NpCl_4$
0.8789	$YCr_4O_4$	0.9064	$ScVO_4$
0.8794	$PrVO_4$	0.9067	$HfSi_4O_4$
0.8796	$ErCr_4O_4$	0.9095	$PaGe_4O_4$
0.8796	$CeVO_4$	0.9097	$[ZrSi_4O_4]$
0.8797	$CaBeF_4$	0.9099	$YAs_4O_4$
0.8797	$YVO_4$	0.9110	$ScAs_4O_4$
0.8804	$GdVO_4$	0.9186	$UGe_4O_4$
0.8807	$YbCr_4O_4$	0.9231	$NpGe_4O_4$
0.8811	$ScPO_4$	1.0300	$CuFe_2O_4$
0.8814	$ThCl_4$	1.4142	$Ni_{15}O_{16}$
0.8817	$(Ta, Nb)BO_4$	1.4670	$NiRh_2O_4$
0.8817	$GdVO_4$	1.4715	$SrPb_2I_6 \cdot 7H_2O$
0.8819	$EuVO_4$	1.5592	$(Mn, Fe)_3O_4$
0.8823	$LuCr_4O_4$	1.5707	$ZnHMn_{1.6}O_4$
0.8825	$TbVO_4$	1.5832	$Zn_4(Mn, Zn, Si)_8O_{16} \cdot 2H_2O$
0.8828	$TaBO_4$	1.5839	$CaIn_2O_4$
0.8830	$LuVO_4$	1.6146	$CdIn_2O_4$
0.8831	$DyVO_4$	1.6181	$ZnMn_2O_4$
0.8831	$YVO_4$	1.6195	$MgMn_2O_4$
0.8840	$ErVO_4$	1.6211	$MgMn_2O_4$
0.8840	$BiVO_4$	1.6383	$Mn_3O_4$
0.8845	$ThSi_4O_4$	1.6410	$Mn_3O_4$
0.8849	$YbVO_4$	1.6765	$BaU_2O_7$
0.8853	$HoVO_4$	1.6947	$(Cu_{1-2x}Cu_{2x})_2O_{1-x}$
0.8855	$ThSi_4O_4$	1.6988	$CdMn_2O_4$
0.8857	$TmVO_4$	2.0187	$(NH_4)_2SbBr_6$

I4<sub>1</sub>/amd D<sub>4h</sub><sup>19</sup> No. 141 (continued)

## Inorganic (continued)

2.1580	Li <sub>2</sub> Fe <sub>2</sub> Cl <sub>4</sub>	3.2960	NdSi <sub>2</sub>
2.1610	LiFeCl <sub>2</sub>	3.2996	Si <sub>2</sub> Sm
2.1659	LiInCl <sub>2</sub>	3.3014	Ge <sub>2</sub> Sm
2.1993	[PbMoCl <sub>4</sub> ]	3.3113	Si <sub>2</sub> Sm
2.2147	LiScCl <sub>2</sub>	3.3166	CeSi <sub>2</sub>
2.2597	NaGdCl <sub>2</sub>	3.3195	GdSi <sub>2</sub>
2.2970	PbU	3.3201	DySi <sub>2</sub>
2.4120	Ni(CN) <sub>2</sub> •NH <sub>3</sub>	3.3218	Si <sub>2</sub> Y
2.4131	LiYCl <sub>2</sub>	3.3301	GdGe <sub>2</sub>
2.4836	PbTh	3.3374	GdGe <sub>1.67</sub>
2.5121	TiCl <sub>2</sub>	3.3686	CeGe <sub>2</sub>
2.5136	TiCl <sub>2</sub>	3.3702	Ge <sub>2</sub> Y
2.8341	Li <sub>6</sub> BeF <sub>4</sub> ZrF <sub>8</sub>	3.3744	DyGe <sub>1.67</sub>
2.8940	UCl <sub>3</sub>	3.3892	DyGe <sub>1.62</sub>
3.0000	Sb <sub>6</sub> Cl <sub>13</sub>	3.4121	PuSi <sub>2</sub>
3.1636	Si <sub>3</sub> Sr <sub>2</sub>	3.4509	NpSi <sub>2</sub>
3.1841	EuSi <sub>2</sub>	3.4523	Si <sub>2</sub> U
3.2116	LaSi <sub>2</sub>	3.4566	Ge <sub>2</sub> Th
3.2762	PrSi <sub>2</sub>	3.4622	Ge <sub>2</sub> Th
3.2777	Ge <sub>2</sub> Pr	3.4770	Si <sub>2</sub> Th
3.2783	Ge <sub>2</sub> Nd	4.2450	In <sub>2</sub> S <sub>3</sub>
3.2864	Ge <sub>2</sub> La	5.4350	BW
3.2879	CeGe <sub>2</sub>	6.3793	As <sub>3</sub> Ni <sub>11</sub>
3.2917	Ge <sub>2</sub> Nd	7.9047	Al <sub>4</sub> Si <sub>5</sub> Zr <sub>3</sub>
3.2956	PrSi <sub>2</sub>		

## Organic

0.541	Pt(C <sub>7</sub> H <sub>6</sub> Cl <sub>2</sub> N) <sub>2</sub>	1.358	BaC <sub>4</sub> H <sub>4</sub> Cl <sub>4</sub>
0.7225	Si <sub>5</sub> Cl <sub>6</sub> (CH <sub>3</sub> ) <sub>8</sub>	2.4120	Ni(CN) <sub>2</sub> •NH <sub>3</sub>
0.8474	C <sub>32</sub> H <sub>36</sub> N <sub>4</sub> Ni	4.273	Ce(NH <sub>2</sub> ) <sub>2</sub> •NaBr•H <sub>2</sub> O
0.8522	C <sub>32</sub> H <sub>36</sub> N <sub>4</sub> Ni		

4 2 2  
m m mI4<sub>1</sub>/acd D<sub>4h</sub><sup>20</sup> No. 142Inorganic - 16  
Organic - 4

## Inorganic

0.6667	Ca(Zr, Ca) <sub>2</sub> Zr <sub>4</sub> (Ti, Fe) <sub>2</sub> Cl <sub>16</sub>	1.9749	Mg(H <sub>2</sub> Pd <sub>2</sub> ) <sub>2</sub> •6H <sub>2</sub> O
1.0000	NaAlSi <sub>2</sub> Cl <sub>6</sub> •H <sub>2</sub> O	1.9926	3Mn <sub>2</sub> Cl <sub>3</sub> •MnSiCl <sub>3</sub>
1.0000	CsAlSi <sub>2</sub> Cl <sub>6</sub> •H <sub>2</sub> O	1.9937	CaMn <sub>6</sub> SiCl <sub>12</sub>
1.2778	Fe <sub>2</sub> (TeCl <sub>3</sub> ) <sub>3</sub> •xH <sub>2</sub> O	2.0076	As <sub>2</sub> Zn <sub>3</sub>
1.2803	Fe(OH)(Te <sub>2</sub> Cl <sub>5</sub> )	3.0625	B <sub>20</sub> H <sub>16</sub>
1.6773	NaPb	3.0715	B <sub>20</sub> H <sub>16</sub>
1.8780	C <sub>2</sub> Na <sub>2</sub>	3.7562	PdSn <sub>2</sub>
1.9380	C <sub>2</sub> K <sub>2</sub>	5.9792	Au <sub>3</sub> Zn

## Organic

1.070	Ni(NC <sub>5</sub> H <sub>5</sub> ) <sub>4</sub> Cl <sub>2</sub>	1.8780	Na <sub>2</sub> C <sub>2</sub>
1.2838	(CH <sub>3</sub> ) <sub>2</sub> C(COOH) <sub>2</sub>	1.9380	K <sub>2</sub> C <sub>2</sub>

3

P3 C<sub>3</sub><sup>1</sup> No. 143Inorganic - 4  
Organic - 4

## Inorganic

0.9420	LiBCl <sub>2</sub> •8H <sub>2</sub> O	1.5670	Zn <sub>4</sub> (OH) <sub>5</sub> Cl(SO <sub>4</sub> )•1.6H <sub>2</sub> O
0.9473	Cu <sub>2</sub> SiS <sub>3</sub>	3.8728	Fe <sub>8</sub> Pb <sub>24</sub> Si <sub>27</sub> Cl <sub>84</sub> (OH, Cl) <sub>8</sub>

## Organic

0.2053	(CH <sub>3</sub> CC <sub>6</sub> H <sub>4</sub> ) <sub>3</sub> C•ClCl <sub>4</sub>	0.3904	3C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub> •CH <sub>3</sub> CN
0.3405	C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub>	0.9690	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> CBr

3		$P3_1$	$C_3^2$	No. 144 (includes $P3_2$ No. 145)		Inorganic - 22
						Organic - 8
Inorganic						
0.5835	NaLuF <sub>4</sub>			0.6124	NaPuF <sub>4</sub>	
0.5840	NaYbF <sub>4</sub>			0.6128	NaPrF <sub>4</sub>	
0.5862	NaTmF <sub>4</sub>			0.6132	NaPuF <sub>4</sub>	
0.5901	NaErF <sub>4</sub>			0.6150	NaCeF <sub>4</sub>	
0.5906	NaYF <sub>4</sub>			0.6187	K <sub>2</sub> UF <sub>6</sub>	
0.5921	NaHoF <sub>4</sub>			0.6197	NaLaF <sub>4</sub>	
0.5941	NaDyF <sub>4</sub>			0.6296	Na <sub>2</sub> UF <sub>6</sub>	
0.5993	NaGdF <sub>4</sub>			0.6403	Na <sub>2</sub> ThF <sub>6</sub>	
0.6013	NaEuF <sub>4</sub>			1.9229	B <sub>2</sub> O <sub>3</sub>	
0.6032	NaSmF <sub>4</sub>			2.4411	Fe <sub>7</sub> Se <sub>8</sub>	
0.6107	NaAmF <sub>4</sub>			12.0850	(Mg,Al) <sub>3</sub> (Si,Al) <sub>2</sub> (OH) <sub>5</sub> (OH) <sub>4</sub>	
Organic						
0.283	C <sub>10</sub> H <sub>19</sub> O <sub>8</sub> H			0.8468	(NH <sub>2</sub> ) <sub>2</sub> CSe	
0.5411	C <sub>14</sub> H <sub>23</sub> ClO <sub>2</sub>			0.9750	C <sub>7</sub> H <sub>14</sub> O <sub>5</sub>	
0.6211	CH <sub>2</sub> =CH-CO-NH-CO-NH-CO-C <sub>6</sub> H <sub>5</sub>			4.315	C <sub>37</sub> H <sub>38</sub> MgN <sub>4</sub> O <sub>5</sub> •H <sub>2</sub> O	
0.7784	CH <sub>2</sub> NH <sub>2</sub> COOH			8.1409	C <sub>19</sub> H <sub>26</sub> O <sub>3</sub>	

3		$P3_2$	$C_3^3$	No. 145 (see No. 144)		
.....						
3		R3	$C_3^4$	No. 146		Inorganic - 20
						Organic - 15
Inorganic						
0.6690	LiZnV <sub>4</sub>			1.0674	Ga <sub>5</sub> V	
0.6702	LiZnAs <sub>4</sub>			1.2365	CsGeCl <sub>3</sub>	
0.6834	Cu <sub>6</sub> Zn <sub>3</sub> As <sub>4</sub> S <sub>12</sub>			1.4893	Tl <sub>2</sub> S	
0.9974	MgSeO <sub>3</sub> •6H <sub>2</sub> O			2.1883	NaIO <sub>4</sub> •3H <sub>2</sub> O	
0.9991	MgSeO <sub>3</sub> •6H <sub>2</sub> O			2.3573	Fe <sub>3</sub> K(SO <sub>4</sub> ) <sub>2</sub> (OH) <sub>6</sub>	
1.0241	MgHP <sub>3</sub> •6H <sub>2</sub> O			2.9170	CrCl <sub>3</sub>	
1.0247	CoSO <sub>3</sub> •6H <sub>2</sub> O			4.9122	InMg <sub>3</sub>	
1.0261	MgSO <sub>3</sub> •6H <sub>2</sub> O			6.7247	Fe <sub>4</sub> Fe <sub>2</sub> (OH) <sub>8</sub> Fe <sub>2</sub> Si <sub>2</sub> O <sub>10</sub>	
1.0271	NiSO <sub>3</sub> •6H <sub>2</sub> O			9.7336	3CeFCO <sub>3</sub> •2CaCO <sub>3</sub>	
1.0313	NiSO <sub>3</sub> •6H <sub>2</sub> O			11.7210	2CeFCO <sub>3</sub> •CaCO <sub>3</sub>	
Organic						
0.1839	(CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> ) <sub>3</sub> COHCl <sub>2</sub> •4H <sub>2</sub> O			0.5269	BiCl <sub>3</sub> •3SC(NH <sub>2</sub> ) <sub>2</sub>	
0.1839	(CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> ) <sub>3</sub> COHBr <sub>2</sub> •4H <sub>2</sub> O			0.5372	Zn <sub>4</sub> [S <sub>2</sub> P(OC <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> ] <sub>6</sub> O	
0.2049	CHI <sub>3</sub> •3C <sub>9</sub> H <sub>7</sub> N			0.5487	BiCl <sub>3</sub> •(C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> S) <sub>3</sub>	
0.2432	(C <sub>6</sub> H <sub>5</sub> -C≡C-) <sub>3</sub> Sb			1.0829	C <sub>19</sub> H <sub>24</sub> N <sub>2</sub> O	
0.2462	(C <sub>6</sub> H <sub>5</sub> -C≡C-) <sub>3</sub> As			1.185	(NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub> COH	
0.2503	(C <sub>6</sub> H <sub>5</sub> -C≡C-) <sub>3</sub> P			9.733	3CeFCO <sub>3</sub> •2CaCO <sub>3</sub>	
0.2657	(H <sub>2</sub> C:CH•C <sub>5</sub> H <sub>4</sub> N) <sub>3</sub>			11.721	2CeFCO <sub>3</sub> •CaCO <sub>3</sub>	
0.335	3C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub> •CH <sub>3</sub> OH					

3		$P\bar{3}$	$C_{3i}^1$	No. 147		Inorganic - 39
						Organic - 7
Inorganic						
0.3693	AgZn			1.3575	K <sub>2</sub> Pb <sub>2</sub> Ge <sub>2</sub> O <sub>7</sub>	
0.4355	Cu <sub>10</sub> Sb <sub>3</sub>			1.3842	Pb <sub>2</sub> Rb <sub>2</sub> Ge <sub>2</sub> O <sub>7</sub>	
0.4968	CaCl <sub>2</sub> •6H <sub>2</sub> O			1.3898	Pb <sub>2</sub> Rb <sub>2</sub> Si <sub>2</sub> O <sub>7</sub>	
0.5041	SrI <sub>2</sub> •6H <sub>2</sub> O			1.4365	Cs <sub>2</sub> Pb <sub>2</sub> Ge <sub>2</sub> O <sub>7</sub>	
0.5049	SrBr <sub>2</sub> •6H <sub>2</sub> O			1.4522	Cs <sub>2</sub> Pb <sub>2</sub> Si <sub>2</sub> O <sub>7</sub>	
0.5060	CaI <sub>2</sub> •6H <sub>2</sub> O			1.5951	Er <sub>4</sub> Cu <sub>6</sub> S <sub>9</sub>	
0.5148	SrCl <sub>2</sub> •6H <sub>2</sub> O			1.5976	Tm <sub>4</sub> Cu <sub>6</sub> S <sub>9</sub>	
0.5169	BaI <sub>2</sub> •6H <sub>2</sub> O			1.5985	Ho <sub>4</sub> Cu <sub>6</sub> S <sub>9</sub>	
0.5568	FeNa <sub>3</sub> (SO <sub>4</sub> ) <sub>3</sub> •3H <sub>2</sub> O			1.5994	Yb <sub>4</sub> Cu <sub>6</sub> S <sub>9</sub>	
0.6069	U <sub>3</sub> O <sub>8</sub>			1.6002	Y <sub>4</sub> Cu <sub>6</sub> S <sub>9</sub>	
1.1272	Na <sub>2</sub> SO <sub>3</sub>			1.6022	Dy <sub>4</sub> Cu <sub>6</sub> S <sub>9</sub>	
1.1632	Mg <sub>2</sub> MnCl <sub>6</sub> •12H <sub>2</sub> O			1.6049	Lu <sub>4</sub> Cu <sub>6</sub> S <sub>9</sub>	
1.1748	CdNi <sub>2</sub> Cl <sub>6</sub> •12H <sub>2</sub> O			1.6201	LuCu <sub>3</sub> S <sub>3</sub>	
1.3412	K <sub>2</sub> Pb <sub>2</sub> Si <sub>2</sub> O <sub>7</sub>			1.6202	Cu <sub>3</sub> YbS <sub>3</sub>	
1.3535	K <sub>2</sub> Pb <sub>2</sub> Si <sub>2</sub> O <sub>7</sub>			1.6291	TmCu <sub>3</sub> S <sub>3</sub>	

P3 C<sub>3i</sub><sup>1</sup> No. 147 (continued)

## Inorganic (continued)

1.6344	ErCu <sub>3</sub> S <sub>3</sub>	1.9239	Ca <sub>2</sub> Si <sub>4</sub> O <sub>10</sub> •H <sub>2</sub> O
1.6380	HoCu <sub>3</sub> S <sub>3</sub>	1.9570	[Ca <sub>14</sub> K(Si <sub>24</sub> O <sub>60</sub> )(OH) <sub>5</sub> •5H <sub>2</sub> O]
1.6391	YCu <sub>3</sub> S <sub>3</sub>	3.3333	MgNa <sub>2</sub> (CO <sub>3</sub> ) <sub>2</sub>
1.6402	DyCu <sub>3</sub> S <sub>3</sub>	7.9066	NW <sub>2</sub>
1.6414	TbCu <sub>3</sub> S <sub>3</sub>		

## Organic

0.2545	C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub>	0.8679	(CH <sub>3</sub> ) <sub>3</sub> SiOSi(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub>
0.6796	Zn(C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O) <sub>6</sub> (ClO <sub>4</sub> ) <sub>2</sub>	0.9427	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> CCL
0.6824	Ca(C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O) <sub>6</sub> (ClO <sub>4</sub> ) <sub>2</sub>	3.333	Na <sub>2</sub> Mg(CO <sub>3</sub> ) <sub>2</sub>
0.6941	Mg(C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O) <sub>6</sub> (ClO <sub>4</sub> ) <sub>2</sub>		

3

R3 C<sub>3i</sub><sup>2</sup> No. 148Inorganic - 226  
Organic - 50

## Inorganic

0.3711	Ag <sup>+</sup> CN	0.9841	KAsF <sub>6</sub>
0.3887	NaBr•5.143NH <sub>3</sub>	0.9878	Cr(NH <sub>3</sub> ) <sub>6</sub> •Mn(CN) <sub>6</sub>
0.3910	NaCl•5.143NH <sub>3</sub>	0.9886	Cr(NH <sub>3</sub> ) <sub>6</sub> •Co(CN) <sub>6</sub>
0.3917	S	0.9889	Co(NH <sub>3</sub> ) <sub>6</sub> •Fe(CN) <sub>6</sub>
0.4819	H <sub>2</sub> O	0.9892	Co(NH <sub>3</sub> ) <sub>6</sub> •Co(CN) <sub>6</sub>
0.5339	Cu <sub>6</sub> Si <sub>6</sub> O <sub>18</sub> •6H <sub>2</sub> O	0.9896	Co(NH <sub>3</sub> ) <sub>5</sub> H <sub>2</sub> O•Cr(CN) <sub>6</sub>
0.6586	Be <sub>2</sub> GeO <sub>4</sub>	0.9927	Co(NH <sub>3</sub> ) <sub>6</sub> •Co(CN) <sub>6</sub>
0.6611	Be <sub>2</sub> SiO <sub>4</sub>	0.9933	KIrF <sub>6</sub>
0.6629	Be <sub>2</sub> SiO <sub>4</sub>	0.9936	Cr(NH <sub>3</sub> ) <sub>6</sub> •Fe(CN) <sub>6</sub>
0.6638	NaUF <sub>5</sub>	0.9958	Co(NH <sub>3</sub> ) <sub>5</sub> H <sub>2</sub> O•Fe(CN) <sub>6</sub>
0.6655	Li <sub>2</sub> MoO <sub>4</sub>	0.9959	Co(NH <sub>3</sub> ) <sub>5</sub> H <sub>2</sub> O•Fe(CN) <sub>6</sub>
0.6660	LiAlSiO <sub>4</sub>	0.9982	Co(NH <sub>3</sub> ) <sub>5</sub> H <sub>2</sub> O•Co(CN) <sub>6</sub>
0.6663	Na <sub>7</sub> Np <sub>6</sub> F <sub>31</sub>	0.9994	KVF <sub>6</sub>
0.6675	Na <sub>7</sub> Am <sub>6</sub> F <sub>31</sub>	0.9994	KOsF <sub>6</sub>
0.6679	Li <sub>2</sub> ZnF <sub>4</sub>	1.0062	FeSiF <sub>6</sub> •6H <sub>2</sub> O
0.6683	LiGaGeO <sub>4</sub>	1.0066	FeSiF <sub>6</sub> •6H <sub>2</sub> O
0.6683	Na <sub>7</sub> Pu <sub>6</sub> F <sub>31</sub>	1.0082	MgTiF <sub>6</sub> •6H <sub>2</sub> O
0.6684	Na <sub>7</sub> Np <sub>6</sub> F <sub>31</sub>	1.0087	MnSiF <sub>6</sub> •6H <sub>2</sub> O
0.6686	Li <sub>2</sub> WO <sub>4</sub>	1.0090	NiSnCl <sub>6</sub> •6H <sub>2</sub> O
0.6695	Na <sub>7</sub> Pu <sub>6</sub> F <sub>31</sub>	1.0093	MnSiF <sub>6</sub> •6H <sub>2</sub> O
0.6696	(Zn,Be) <sub>2</sub> SiO <sub>4</sub>	1.0093	NiSnCl <sub>6</sub> •6H <sub>2</sub> O
0.6697	Zn <sub>2</sub> GeO <sub>4</sub>	1.0095	FeF <sub>3</sub> •3H <sub>2</sub> O
0.6700	Zn <sub>2</sub> SiO <sub>4</sub>	1.0096	CrF <sub>3</sub> •3H <sub>2</sub> O
0.6704	Li <sub>2</sub> BeF <sub>4</sub>	1.0097	NiSnCl <sub>6</sub> •6H <sub>2</sub> O
0.6704	Na <sub>7</sub> Cm <sub>6</sub> F <sub>31</sub>	1.0102	Co(NH <sub>3</sub> ) <sub>5</sub> H <sub>2</sub> O•Co(CN) <sub>6</sub>
0.6705	Li <sub>2</sub> CrO <sub>4</sub>	1.0107	GaF <sub>3</sub> •3H <sub>2</sub> O
0.6714	ALLiGeO <sub>4</sub>	1.0109	CoF <sub>3</sub> •3H <sub>2</sub> O
0.6733	CdAl <sub>2</sub> O <sub>4</sub>	1.0109	AlF <sub>3</sub> •3H <sub>2</sub> O
0.6744	LiNaBeF <sub>4</sub>	1.0130	CoSnCl <sub>6</sub> •6H <sub>2</sub> O
0.6753	KAmF <sub>5</sub>	1.0147	Mg(H <sub>2</sub> O) <sub>6</sub> TeCl <sub>6</sub>
0.6770	(Zn,Mn) <sub>2</sub> SiO <sub>4</sub>	1.0164	MgTiF <sub>6</sub> •6H <sub>2</sub> O
0.6791	NaPuF <sub>5</sub>	1.0164	MgSnCl <sub>6</sub> •6H <sub>2</sub> O
0.6812	NH <sub>4</sub> UF <sub>5</sub>	1.0205	CoSnCl <sub>6</sub> •6H <sub>2</sub> O
0.6812	(NH <sub>4</sub> ) <sub>7</sub> U <sub>6</sub> F <sub>31</sub>	1.0208	MnF <sub>3</sub> •3H <sub>2</sub> O
0.6825	Na <sub>7</sub> Zr <sub>6</sub> F <sub>31</sub>	1.0218	MgSnCl <sub>6</sub> •6H <sub>2</sub> O
0.6825	NH <sub>4</sub> PuF <sub>5</sub>	1.0246	NiPtI <sub>6</sub> •6H <sub>2</sub> O
0.6825	(NH <sub>4</sub> ) <sub>7</sub> Pu <sub>6</sub> F <sub>31</sub>	1.0256	MgSnF <sub>6</sub> •6H <sub>2</sub> O
0.6847	K <sub>7</sub> Th <sub>6</sub> F <sub>31</sub>	1.0259	NiSiF <sub>6</sub> •6H <sub>2</sub> O
0.6850	KThF <sub>5</sub>	1.0269	NiSiF <sub>6</sub> •6H <sub>2</sub> O
0.6861	KUF <sub>5</sub>	1.0272	ZnTiF <sub>6</sub> •6H <sub>2</sub> O
0.6878	K <sub>7</sub> Np <sub>6</sub> F <sub>31</sub>	1.0272	ZnMoO <sub>4</sub> F <sub>5</sub> •6H <sub>2</sub> O
0.6885	K <sub>7</sub> Pu <sub>6</sub> F <sub>31</sub>	1.0272	NiPtBr <sub>6</sub> •6H <sub>2</sub> O
0.6932	KPuF <sub>5</sub>	1.0282	CoPtCl <sub>6</sub> •6H <sub>2</sub> O
0.6964	RbPuF <sub>5</sub>	1.0288	NiSnF <sub>6</sub> •6H <sub>2</sub> O
0.6969	Rb <sub>7</sub> Np <sub>6</sub> F <sub>31</sub>	1.0288	FePtCl <sub>6</sub> •6H <sub>2</sub> O
0.6976	Rb <sub>7</sub> Pu <sub>6</sub> F <sub>31</sub>	1.0314	MnTiF <sub>6</sub> •6H <sub>2</sub> O
0.7104	Mg <sub>7</sub> Na <sub>12</sub> (SO <sub>4</sub> ) <sub>13</sub> •15H <sub>2</sub> O	1.0318	CdMoO <sub>4</sub> F <sub>4</sub> •6H <sub>2</sub> O
0.9262	Zr <sub>7</sub> O <sub>8</sub> N <sub>4</sub>	1.0323	CeOsF <sub>6</sub>
0.9342	U <sub>2</sub> Y <sub>5</sub> O <sub>13.5</sub>	1.0323	MnSnF <sub>6</sub> •6H <sub>2</sub> O
0.9351	U <sub>2</sub> Y <sub>5</sub> O <sub>12</sub>	1.0323	NiPtCl <sub>6</sub> •6H <sub>2</sub> O
0.9395	Lu <sub>6</sub> UO <sub>12</sub>	1.0331	NiSiF <sub>6</sub> •6H <sub>2</sub> O
0.9426	Y <sub>6</sub> UO <sub>12</sub>	1.0332	NiMoO <sub>4</sub> F <sub>4</sub> •6H <sub>2</sub> O
0.9776	Co(NH <sub>3</sub> ) <sub>6</sub> •Cr(CN) <sub>6</sub>	1.0332	ZnMoO <sub>4</sub> F <sub>4</sub> •6H <sub>2</sub> O
0.9812	Cr(NH <sub>3</sub> ) <sub>6</sub> •Cr(CN) <sub>6</sub>	1.0332	CoMoO <sub>4</sub> F <sub>4</sub> •6H <sub>2</sub> O
0.9822	Co(NH <sub>3</sub> ) <sub>6</sub> •Cr(CN) <sub>6</sub>	1.0338	ZnPtCl <sub>6</sub> •6H <sub>2</sub> O

R $\bar{3}$  C $_{3i}^2$  No. 148 (continued)

## Inorganic (continued)

1.0344	MgPtCl <sub>6</sub> •6H <sub>2</sub> O	2.7678	CoTiO <sub>3</sub>
1.0345	MgSiF <sub>6</sub> •6H <sub>2</sub> O	2.7688	TbI <sub>3</sub>
1.0346	ZnTiF <sub>6</sub> •6H <sub>2</sub> O	2.7695	AmI <sub>3</sub>
1.0348	ZnZrF <sub>6</sub> •6H <sub>2</sub> O	2.7709	NiMnO <sub>3</sub>
1.0353	ZnSiF <sub>6</sub> •6H <sub>2</sub> O	2.7709	MgTiO <sub>3</sub>
1.0354	MgSiF <sub>6</sub> •6H <sub>2</sub> O	2.7736	YI <sub>3</sub>
1.0356	ZnSiF <sub>6</sub> •6H <sub>2</sub> O	2.7745	NaUF <sub>6</sub>
1.0356	ZnZrF <sub>6</sub> •6H <sub>2</sub> O	2.7770	SmI <sub>3</sub>
1.0356	NiPdCl <sub>6</sub> •6H <sub>2</sub> O	2.7796	CoMnO <sub>3</sub>
1.0369	NiZrF <sub>6</sub> •6H <sub>2</sub> O	2.7807	MgTiO <sub>3</sub>
1.0369	ZnPdCl <sub>6</sub> •6H <sub>2</sub> O	2.7821	YI <sub>3</sub>
1.0381	ZnSnF <sub>6</sub> •6H <sub>2</sub> O	2.7822	DyI <sub>3</sub>
1.0381	ZnSnF <sub>6</sub> •6H <sub>2</sub> O	2.7851	ScCl <sub>3</sub>
1.0385	ZnNbOF <sub>5</sub> •6H <sub>2</sub> O	2.7853	HoI <sub>3</sub>
1.0385	MnSnCl <sub>6</sub> •6H <sub>2</sub> O	2.7872	YbI <sub>3</sub>
1.041	MgSnF <sub>6</sub> •6H <sub>2</sub> O	2.7889	ErI <sub>3</sub>
1.0413	CdSnF <sub>6</sub> •6H <sub>2</sub> O	2.7928	SbI <sub>3</sub>
1.0413	MgPdCl <sub>6</sub> •6H <sub>2</sub> O	2.7961	MnTiO <sub>3</sub>
1.0413	Co(NH <sub>3</sub> ) <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub> •Co(CN) <sub>6</sub>	2.8005	LuI <sub>3</sub>
1.0414	CoSiF <sub>6</sub> •6H <sub>2</sub> O	2.8024	TmI <sub>3</sub>
1.0416	CoSiF <sub>6</sub> •6H <sub>2</sub> O	2.8035	Cr <sub>2</sub> S <sub>3</sub>
1.0441	CuPtCl <sub>6</sub> •6H <sub>2</sub> O	2.8339	TiCl <sub>3</sub>
1.0470	CdPtCl <sub>6</sub> •6H <sub>2</sub> O	2.8364	CdTiO <sub>3</sub>
1.0532	CoSnF <sub>6</sub> •6H <sub>2</sub> O	2.8405	CdTiO <sub>3</sub>
1.0622	MnPtCl <sub>6</sub> •6H <sub>2</sub> O	2.8590	TiCl <sub>3</sub>
1.0788	CuSiF <sub>6</sub> •6H <sub>2</sub> O	2.8660	FeBr <sub>3</sub>
1.0850	MnSnCl <sub>6</sub> •6H <sub>2</sub> O	2.8687	NaBiO <sub>3</sub> •xH <sub>2</sub> O
1.0985	KPF <sub>6</sub>	2.8729	FeCl <sub>3</sub>
1.6134	(NH <sub>4</sub> ) <sub>2</sub> H <sub>3</sub> I <sub>6</sub>	2.8842	VCl <sub>3</sub>
1.6819	(HSi <sub>1.5</sub> ) <sub>8</sub>	2.8950	TiBr <sub>3</sub>
1.7636	Mn <sub>6</sub> Si	2.9380	K <sub>4</sub> Ni(N <sub>2</sub> ) <sub>6</sub>
1.7783	Co-Mn-Si	2.9708	AsI <sub>3</sub>
1.8496	Na <sub>2</sub> H <sub>4</sub> O <sub>7</sub> •5H <sub>2</sub> O	3.0004	NaSbO <sub>3</sub>
1.9525	K <sub>2</sub> Sn(OH) <sub>6</sub>	3.1310	Tl <sub>4</sub> Ni(N <sub>2</sub> ) <sub>6</sub>
2.0016	K <sub>2</sub> Pt(OH) <sub>6</sub>	3.1436	Ce <sub>2</sub> Mg <sub>3</sub> (N <sub>2</sub> ) <sub>12</sub> •24H <sub>2</sub> O
2.0476	2NH <sub>4</sub> Cl•(NH <sub>4</sub> ) <sub>4</sub> Fe(CN) <sub>6</sub>	3.1600	NiSn(B <sub>2</sub> ) <sub>2</sub>
2.0574	Ag <sub>2</sub> H <sub>3</sub> I <sub>6</sub>	3.1672	CoSn(B <sub>2</sub> ) <sub>2</sub>
2.1405	Ag <sub>2</sub> H <sub>3</sub> I <sub>6</sub>	3.1718	MgSn(B <sub>2</sub> ) <sub>2</sub>
2.2897	(K,Fe) <sub>2</sub> Na <sub>4</sub> O <sub>8</sub> (SO <sub>4</sub> ) <sub>3</sub> •5H <sub>2</sub> O	3.2077	MnSn(B <sub>2</sub> ) <sub>2</sub>
2.3732	Na <sub>2</sub> Sn(OH) <sub>6</sub>	3.2393	CdSn(B <sub>2</sub> ) <sub>2</sub>
2.3815	Na <sub>2</sub> Sn(OH) <sub>6</sub>	3.2811	CaSn(B <sub>2</sub> ) <sub>2</sub>
2.5334	AlF <sub>3</sub>	3.2970	Ca(Mg,Fe,Mn)(C <sub>2</sub> ) <sub>2</sub>
2.6255	LiSbF <sub>6</sub>	3.3184	CaSn(B <sub>2</sub> ) <sub>2</sub>
2.6930	Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	3.3299	CaMg(C <sub>2</sub> ) <sub>2</sub>
2.7045	LiNbO <sub>3</sub>	3.3393	Ca <sub>3</sub> (Mg <sub>2</sub> Fe)(C <sub>2</sub> ) <sub>6</sub>
2.7206	FeRhO <sub>3</sub>	3.3680	CaK <sub>2</sub> (C <sub>2</sub> ) <sub>2</sub>
2.7354	CrRhO <sub>3</sub>	3.3691	CaMn(C <sub>2</sub> ) <sub>2</sub>
2.7376	WCl <sub>6</sub>	3.3936	SrSn(B <sub>2</sub> ) <sub>2</sub>
2.7399	NiTiO <sub>3</sub>	3.3971	KShO <sub>3</sub>
2.7419	CrI <sub>3</sub>	3.4835	BaSn(B <sub>2</sub> ) <sub>2</sub>
2.7444	CdSnO <sub>3</sub>	3.6209	KAu(CN) <sub>2</sub>
2.7455	MgTiO <sub>3</sub>	4.0571	TlSbO <sub>3</sub>
2.7474	NiTiO <sub>3</sub>	4.3402	SrGeO <sub>3</sub>
2.7488	CoTiO <sub>3</sub>	4.4116	(Mn,Mg) <sub>13</sub> (Al,Fe) <sub>2</sub> As(AsO <sub>4</sub> ) <sub>2</sub> (OH) <sub>21</sub> O <sub>4</sub>
2.7498	MgTiO <sub>3</sub>	4.6927	Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> •9H <sub>2</sub> O
2.7533	BiI <sub>3</sub>	4.9493	NaTmO <sub>2</sub>
2.7601	FeTiO <sub>3</sub>	4.9775	CHO <sub>2</sub>
2.7630	GdI <sub>3</sub>	5.5324	FeTiO <sub>3</sub>

## Organic

0.1082	C <sub>2</sub> H <sub>5</sub> O•C <sub>6</sub> H <sub>4</sub> CH:CH•C <sub>6</sub> H <sub>5</sub>	0.3711	Ag <sub>2</sub> CN
0.2945	C <sub>11</sub> H <sub>11</sub> IN <sub>2</sub> O	0.6249	C <sub>38</sub> H <sub>46</sub> O <sub>6</sub> N <sub>4</sub>
0.2947	C <sub>11</sub> H <sub>11</sub> BrN <sub>2</sub> O	0.7927	[Fe(NH <sub>2</sub> C <sub>6</sub> NH <sub>2</sub> ) <sub>6</sub> ]Cl <sub>3</sub> •3H <sub>2</sub> O
0.3278	C <sub>6</sub> (CH <sub>2</sub> Br) <sub>6</sub>	0.8054	Sb(S•CS•O•C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub>
0.328	3C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub> •C <sub>2</sub> H <sub>2</sub>	0.8888	Cr(SCS <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub>
0.3293	C <sub>14</sub> H <sub>28</sub> N <sub>2</sub> NiS <sub>4</sub>	0.8902	Fe(S-CS-O-C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub>
0.330	3C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub> •HCl	0.905	Co(SCS <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub>
0.331	3C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub> •HBr	0.9776	Co(NH <sub>3</sub> ) <sub>6</sub> •Cr(CN) <sub>6</sub>
0.331	3C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub> •H <sub>2</sub> S	0.9812	Cr(NH <sub>3</sub> ) <sub>6</sub> •Cr(CN) <sub>6</sub>
0.344	3C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub> •(HCOOH)	0.9822	Co(NH <sub>3</sub> ) <sub>6</sub> •Cr(CN) <sub>6</sub>
0.3469	ClC <sub>6</sub> H <sub>4</sub> SO <sub>2</sub> NHC <sub>6</sub> H <sub>4</sub> Br	0.9878	Cr(NH <sub>3</sub> ) <sub>6</sub> •Mn(CN) <sub>6</sub>
0.357	3C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub> •SO <sub>2</sub>	0.9886	Cr(NH <sub>3</sub> ) <sub>6</sub> •Co(CN) <sub>6</sub>
0.360	3C <sub>6</sub> H <sub>4</sub> (OH) <sub>2</sub> •CO <sub>2</sub>	0.9889	Co(NH <sub>3</sub> ) <sub>6</sub> •Fe(CN) <sub>6</sub>

R $\bar{3}$  C $\bar{3}_i$  No. 148 (continued)

## Organic (continued)

0.9892	Co(NH $\bar{3}$ ) $\bar{6}$ •Co(CN) $\bar{6}$	1.0724	(C $\bar{3}$ H $\bar{7}$ Si $\bar{6}$ 1.5) $\bar{8}$
0.9896	Co(NH $\bar{3}$ ) $\bar{5}$ H $\bar{2}$ •Cr(CN) $\bar{6}$	1.5628	(CH $\bar{3}$ •C $\bar{6}$ H $\bar{4}$ ) $\bar{3}$ As
0.9927	Co(NH $\bar{3}$ ) $\bar{6}$ •Co(CN) $\bar{6}$	1.5790	C $\bar{6}$ H $\bar{3}$ •H•CH $\bar{3}$ •CH•(CH $\bar{3}$ ) $\bar{2}$
0.9936	Cr(NH $\bar{3}$ ) $\bar{6}$ •Fe(CN) $\bar{6}$	1.8631	C $\bar{8}$ H $\bar{8}$
0.9958	Co(NH $\bar{3}$ ) $\bar{5}$ H $\bar{2}$ •Fe(CN) $\bar{6}$	2.048	2NH $\bar{4}$ Cl•(NH $\bar{4}$ ) $\bar{4}$ Fe(CN) $\bar{6}$
0.9959	Co(NH $\bar{3}$ ) $\bar{5}$ H $\bar{2}$ •Fe(CN) $\bar{6}$	2.7256	2Al(C $\bar{2}$ H $\bar{5}$ ) $\bar{3}$ •KF
0.9961	(C $\bar{3}$ H $\bar{7}$ Si $\bar{6}$ 1.5) $\bar{8}$	3.297	Ca(Mg, Fe, Mn)(C $\bar{6}$ ) $\bar{2}$
0.9982	Co(NH $\bar{3}$ ) $\bar{5}$ H $\bar{2}$ •Co(CN) $\bar{6}$	3.3393	Ca $\bar{3}$ (Mg $\bar{2}$ Fe)(C $\bar{6}$ ) $\bar{6}$
1.0102	Co(NH $\bar{3}$ ) $\bar{5}$ H $\bar{2}$ •Co(CN) $\bar{6}$	3.3691	CaMn(C $\bar{6}$ ) $\bar{2}$
1.036	(C $\bar{2}$ H $\bar{5}$ Si $\bar{6}$ 1.5) $\bar{8}$	3.3829	CaK $\bar{2}$ (C $\bar{6}$ ) $\bar{2}$
1.0413	Co(NH $\bar{3}$ ) $\bar{4}$ (H $\bar{2}$ •) $\bar{2}$ •Co(CN) $\bar{6}$	3.6209	KAu(CN) $\bar{2}$
1.0471	(CH $\bar{3}$ Si $\bar{6}$ 1.5) $\bar{8}$	4.9775	Ho $\bar{2}$ C

3 2

P312 D $\bar{3}$  No. 149Inorganic - 18  
Organic - 0

## Inorganic

0.9125	HgSb $\bar{2}$ • $\bar{6}$	1.0154	SrSb $\bar{2}$ • $\bar{6}$
0.9155	CdSb $\bar{2}$ • $\bar{6}$	1.0292	HgAs $\bar{2}$ • $\bar{6}$
0.9209	Fe $\bar{2}$ N	1.0521	CaAs $\bar{2}$ • $\bar{6}$
0.9427	CoAs $\bar{2}$ • $\bar{6}$	1.0855	BaSb $\bar{2}$ • $\bar{6}$
0.9538	UV $\bar{2}$ • $\bar{6}$	1.1144	SrAs $\bar{2}$ • $\bar{6}$
0.9594	CaSb $\bar{2}$ • $\bar{6}$	1.1280	PbAs $\bar{2}$ • $\bar{6}$
0.9942	LaTiSb• $\bar{6}$	1.2075	KNiI• $\bar{6}$
1.0077	CdAs $\bar{2}$ • $\bar{6}$	1.2703	AlF $\bar{3}$
1.0146	PbSb $\bar{2}$ • $\bar{6}$	3.9747	Fe $\bar{4}$ Pb• $\bar{7}$

## Organic

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3 2

P321 D $\bar{3}$  No. 150Inorganic - 47  
Organic - 2

## Inorganic

0.4083	BaGe $\bar{4}$ • $\bar{9}$	1.7223	FeNH $\bar{4}$ (S $\bar{6}$ ) $\bar{2}$
0.4924	CaCl $\bar{2}$ •6H $\bar{2}$ • $\bar{6}$	1.7314	AlNH $\bar{4}$ (Se $\bar{4}$ ) $\bar{2}$
0.4934	CaBr $\bar{2}$ •6H $\bar{2}$ • $\bar{6}$	1.7317	GaNH $\bar{4}$ (Se $\bar{4}$ ) $\bar{2}$
0.5006	CaCl $\bar{2}$ •6H $\bar{2}$ • $\bar{6}$	1.7343	GaTl(S $\bar{6}$ ) $\bar{2}$
0.5053	SrBr $\bar{2}$ •6H $\bar{2}$ • $\bar{6}$	1.7378	GaRb(S $\bar{6}$ ) $\bar{2}$
0.5075	GePd $\bar{2}$	1.7394	AlTl(S $\bar{6}$ ) $\bar{2}$
0.5173	SrCl $\bar{2}$ •6H $\bar{2}$ • $\bar{6}$	1.7397	CrNH $\bar{4}$ (S $\bar{6}$ ) $\bar{2}$
0.5278	Pd $\bar{2}$ Si	1.7411	AlNH $\bar{4}$ (S $\bar{6}$ ) $\bar{2}$
0.5687	Na $\bar{2}$ SiF $\bar{6}$	1.7458	AlRb(S $\bar{6}$ ) $\bar{2}$
0.5752	Ni $\bar{2}$ P	1.7497	GaNH $\bar{4}$ (S $\bar{6}$ ) $\bar{2}$
0.6318	Rb $\bar{2}$ S $\bar{2}$ • $\bar{6}$	1.7510	GaRb(S $\bar{6}$ ) $\bar{2}$
0.6433	K $\bar{2}$ S $\bar{2}$ • $\bar{6}$	1.7513	CrRb(S $\bar{6}$ ) $\bar{2}$
0.8845	Hg $\bar{2}$ NHBr $\bar{2}$	1.7536	AlNH $\bar{4}$ (S $\bar{6}$ ) $\bar{2}$
1.0910	NH $\bar{4}$ [Ni(NH $\bar{3}$ ) $\bar{3}$ (CNS) $\bar{3}$ ]	1.7560	AlRb(S $\bar{6}$ ) $\bar{2}$
1.6915	AlK(S $\bar{6}$ ) $\bar{2}$	1.7604	CrTl(S $\bar{6}$ ) $\bar{2}$
1.6916	FeNH $\bar{4}$ (Se $\bar{4}$ ) $\bar{2}$	1.7607	GaTl(S $\bar{6}$ ) $\bar{2}$
1.6931	FeTl(S $\bar{6}$ ) $\bar{2}$	1.7734	AlTl(S $\bar{6}$ ) $\bar{2}$
1.6952	CrK(S $\bar{6}$ ) $\bar{2}$	1.7902	CsFe(S $\bar{6}$ ) $\bar{2}$
1.6955	AlK(S $\bar{6}$ ) $\bar{2}$	1.7966	CsFe(S $\bar{6}$ ) $\bar{2}$
1.6985	CrK(S $\bar{6}$ ) $\bar{2}$	1.8078	Li $\bar{7}$ Pb $\bar{2}$
1.7072	FeRb(S $\bar{6}$ ) $\bar{2}$	1.8401	CrCs(S $\bar{6}$ ) $\bar{2}$
1.7134	FeNH $\bar{4}$ (S $\bar{6}$ ) $\bar{2}$	1.8528	CsGa(S $\bar{6}$ ) $\bar{2}$
1.7167	FeRb(S $\bar{6}$ ) $\bar{2}$	1.8535	AlCs(S $\bar{6}$ ) $\bar{2}$
1.7210	FeTl(S $\bar{6}$ ) $\bar{2}$		

## Organic

1.0910	NH $\bar{4}$ [Ni(NH $\bar{3}$ ) $\bar{3}$ (CNS) $\bar{3}$ ]	1.288	Cu(C $\bar{10}$ H $\bar{14}$ N $\bar{6}$ ) $\bar{2}$ •0.667(C $\bar{6}$ H $\bar{6}$ )
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3 2	P3 <sub>1</sub> 12	D <sub>3</sub> <sup>3</sup>	No. 151 (includes P3 <sub>2</sub> 12 No. 153)	Inorganic - 11 Organic - 0
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Inorganic				
0.7109	RbN <sub>3</sub>		3.4852	(Ca, Mg, RE) <sub>3</sub> Si <sub>2</sub> ( $\sigma$ , $\sigma$ H, F) <sub>9</sub>
0.9724	(R, Ca)B(Si, Al, P)( $\sigma$ , $\sigma$ H, F) <sub>5</sub>		5.5414	Ca(Mg, Fe, Al) <sub>3</sub> (Al, Si) <sub>4</sub> $\sigma$ <sub>10</sub> ( $\sigma$ H) <sub>2</sub>
2.7977	Li <sub>2</sub> Sn $\sigma$ <sub>3</sub>		5.6604	KMg <sub>3</sub> ( $\sigma$ H, F) <sub>2</sub> (Al, Si) <sub>4</sub> $\sigma$ <sub>10</sub>
2.8738	CrCl <sub>3</sub>		5.7677	(K, Na, Ca, Ba)(Al, Fe) <sub>2</sub> (AlSi <sub>3</sub> $\sigma$ <sub>10</sub> )( $\sigma$ H) <sub>2</sub>
2.8980	CrI <sub>3</sub>		5.8154	K(Li, Al) <sub>3</sub> (F, $\sigma$ H) <sub>2</sub> (Al, Si) <sub>4</sub> $\sigma$ <sub>10</sub>
2.9645	AlCl <sub>3</sub>			
Organic				
.....				
3 2	P3 <sub>1</sub> 21	D <sub>3</sub> <sup>4</sup>	No. 152 (includes P3 <sub>2</sub> 21 No. 154)	Inorganic - 30 Organic - 14
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Inorganic				
0.6446	(NH <sub>4</sub> ) <sub>3</sub> Tc <sub>2</sub> Cl <sub>8</sub> •2H <sub>2</sub> $\sigma$		1.3302	Te
0.9054	SmP $\sigma$ <sub>4</sub> •0.5H <sub>2</sub> $\sigma$		1.4048	Hg <sub>3</sub> $\sigma$ <sub>2</sub> Cr $\sigma$ <sub>4</sub>
0.9084	PmP $\sigma$ <sub>4</sub> •0.5H <sub>2</sub> $\sigma$		1.4092	Hg <sub>3</sub> $\sigma$ <sub>2</sub> Se $\sigma$ <sub>4</sub>
0.9090	NdP $\sigma$ <sub>4</sub> •0.5H <sub>2</sub> $\sigma$		1.4196	Hg <sub>3</sub> $\sigma$ <sub>2</sub> S $\sigma$ <sub>4</sub>
0.9128	NdP $\sigma$ <sub>4</sub> •0.5H <sub>2</sub> $\sigma$		1.8594	CaS $\sigma$ <sub>4</sub> •0.5H <sub>2</sub> $\sigma$
0.9150	SmP $\sigma$ <sub>4</sub> •0.5H <sub>2</sub> $\sigma$		2.2148	AlP $\sigma$ <sub>4</sub>
0.9172	GdP $\sigma$ <sub>4</sub> •0.5H <sub>2</sub> $\sigma$		2.2173	AlP $\sigma$ <sub>4</sub>
0.9274	BiP $\sigma$ <sub>4</sub> •0.5H <sub>2</sub> $\sigma$		2.2175	AlP $\sigma$ <sub>4</sub>
0.9795	CeBSi $\sigma$ <sub>5</sub>		2.2269	HgSe
1.0986	Si $\sigma$ <sub>2</sub>		2.2306	AlAs $\sigma$ <sub>4</sub>
1.1001	Si $\sigma$ <sub>2</sub>		2.2450	N <sub>2</sub> H <sub>4</sub> •H <sub>2</sub> $\sigma$
1.1316	BaZn $\sigma$ <sub>2</sub>		2.2542	GaP $\sigma$ <sub>4</sub>
1.1360	Ge $\sigma$ <sub>2</sub>		2.2916	HgS
1.1367	Se		2.4269	Hg $\sigma$
1.1441	BaZn $\sigma$ <sub>2</sub>		3.0492	RbTh <sub>6</sub> F <sub>25</sub>
Organic				
0.6480	Fe(C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> ) <sub>3</sub> Sb <sub>2</sub> (C <sub>4</sub> H <sub>2</sub> $\sigma$ <sub>6</sub> ) <sub>2</sub> •8H <sub>2</sub> $\sigma$		1.7952	K <sub>3</sub> Rh(C $\sigma$ $\sigma$ ) <sub>6</sub> •H <sub>2</sub> $\sigma$
0.9259	[Co(CNCH <sub>3</sub> ) <sub>5</sub> ]Cl $\sigma$ <sub>4</sub>		1.840	(CH $\sigma$ H-C $\sigma$ $\sigma$ Rb) <sub>2</sub>
0.9453	K <sub>3</sub> Ir(C <sub>2</sub> $\sigma$ <sub>4</sub> ) <sub>3</sub> •2H <sub>2</sub> $\sigma$		2.1824	2C <sub>33</sub> H <sub>36</sub> $\sigma$ <sub>6</sub> •C <sub>6</sub> H <sub>6</sub>
1.0959	BaMo $\sigma$ <sub>2</sub> $\sigma$ <sub>4</sub> (C <sub>2</sub> $\sigma$ <sub>4</sub> ) <sub>2</sub> •5H <sub>2</sub> $\sigma$		2.1923	C <sub>12</sub> H <sub>8</sub> S <sub>2</sub>
1.341	Ni[SC(CH <sub>3</sub> )NH <sub>2</sub> ] <sub>2</sub> (NCS) <sub>2</sub>		3.5384	C <sub>9</sub> H <sub>12</sub> N <sub>4</sub> $\sigma$ <sub>3</sub> Cu•2H <sub>2</sub> $\sigma$
1.636	C <sub>6</sub> H <sub>5</sub> •C $\sigma$ $\sigma$ •C $\sigma$ $\sigma$ •C <sub>6</sub> H <sub>5</sub>		4.2930	Pb(C <sub>6</sub> H <sub>11</sub> $\sigma$ <sub>7</sub> ) <sub>2</sub>
1.7815	K <sub>3</sub> Rh(C <sub>2</sub> $\sigma$ <sub>4</sub> ) <sub>3</sub> •2H <sub>2</sub> $\sigma$		4.3327	C <sub>15</sub> H <sub>17</sub> Br $\sigma$ <sub>6</sub>
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3 2	P3 <sub>2</sub> 12	D <sub>3</sub> <sup>5</sup>	No. 153 (see No. 151)	
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.....				
-----				
3 2	P3 <sub>2</sub> 21	D <sub>3</sub> <sup>6</sup>	No. 154 (see No. 152)	
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.....				
-----				
3 2	R32	D <sub>3</sub> <sup>7</sup>	No. 155	Inorganic - 25 Organic - 7
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Inorganic				
0.7719	Al <sub>3</sub> Er(B $\sigma$ <sub>3</sub> ) <sub>4</sub>		0.7830	Al <sub>3</sub> Sm(B $\sigma$ <sub>3</sub> ) <sub>4</sub>
0.7770	(NH <sub>4</sub> ) <sub>6</sub> MnMo $\sigma$ <sub>3</sub> $\sigma$ <sub>32</sub> •8H <sub>2</sub> $\sigma$		0.7945	Cr <sub>3</sub> Gd(B $\sigma$ <sub>3</sub> ) <sub>4</sub>
0.7780	Al <sub>3</sub> Ho(B $\sigma$ <sub>3</sub> ) <sub>4</sub>		0.8228	Mg <sub>3</sub> Ca(C $\sigma$ <sub>3</sub> ) <sub>4</sub>
0.7786	Al <sub>3</sub> Yb(B $\sigma$ <sub>3</sub> ) <sub>4</sub>		1.2029	Ni <sub>3</sub> Se <sub>2</sub>
0.7793	Al <sub>3</sub> Dy(B $\sigma$ <sub>3</sub> ) <sub>4</sub>		1.2382	ScF <sub>3</sub>
0.7796	Al <sub>3</sub> Y(B $\sigma$ <sub>3</sub> ) <sub>4</sub>		1.2435	Ni <sub>3</sub> S <sub>2</sub>
0.7798	Al <sub>3</sub> Tb(B $\sigma$ <sub>3</sub> ) <sub>4</sub>		1.3693	(Mo, Cr) <sub>2</sub> $\sigma$ <sub>3</sub>
0.7802	Al <sub>3</sub> Gd(B $\sigma$ <sub>3</sub> ) <sub>4</sub>		1.3746	(W, Cr) <sub>2</sub> $\sigma$ <sub>3</sub>
0.7807	Al <sub>3</sub> Eu(B $\sigma$ <sub>3</sub> ) <sub>4</sub>		1.6550	K <sub>3</sub> Cu(CN) <sub>4</sub>
0.7813	Al <sub>3</sub> Y(B $\sigma$ <sub>3</sub> ) <sub>4</sub>		1.7844	K <sub>3</sub> Ag(CN) <sub>4</sub>
0.7829	Al <sub>3</sub> Nd(B $\sigma$ <sub>3</sub> ) <sub>4</sub>		1.7883	K <sub>3</sub> Cu(CN) <sub>4</sub>

R32  $D_3^7$  No. 155 (continued)

## Inorganic (continued)

2.5356  $AlF_3$  3.3367  $BaMg(CO_3)_2$   
 2.5377  $CrF_3$

## Organic

0.8228  $Mg_3Ca(CO_3)_4$  2.0479  $C_{64}H_{90}N_{12}O_{16}$   
 1.655  $K_3[Cu(CN)_4]$  2.9202  $Na_3Nd(O_2CCH_2OCH_2CO)_3 \cdot 6H_2O$   
 1.7844  $K_3Ag(CN)_4$  3.3367  $BaMg(CO_3)_2$   
 1.7883  $K_3Cu(CN)_4$

3 m

P3m1  $C_{3v}^1$  No. 156Inorganic - 19  
Organic - 4

## Inorganic

0.6668  $Cd(ClO_4)_2 \cdot 6H_2O$  9.6722  $CdI_2$   
 1.3061  $(Al_{0.76}Fe_{0.02}Fe_{1.73}Mg_{0.16}Ti_{0.15})(Al_{0.76}Si_{1.24})O_5(OH)_4$  11.2842  $CdI_2$   
 15.5395  $CSi$   
 2.4497  $LiK_2AlF_6$  17.7311  $CdI_2$   
 4.5945  $PbI_2$  20.9434  $CdI_2$   
 4.8361  $CdI_2$  20.9434  $CdI_2$   
 4.9082  $CuI$  22.0838  $CSi$   
 6.4481  $CdI_2$  22.5684  $CdI_2$   
 8.0601  $CdI_2$  29.4509  $CSi$   
 8.1793  $CSi$  40.3302  $CdI_2$

## Organic

8.178  $SiC$  22.08  $SiC$   
 15.5395  $SiC$  29.4509  $SiC$

3 m

P31m  $C_{3v}^2$  No. 157Inorganic - 6  
Organic - 3

## Inorganic

0.5751  $K_3V_5O_{14}$  0.8661  $Na_2ZnCl_4 \cdot 3H_2O$   
 0.7062  $RbNO_3$  1.0823  $Ag_5Pb_2O_6$   
 0.7139  $CsNO_3$  2.0871  $Na_2CaBa_4RE_{1.5}Sr_{0.2}U_{0.3}(CO_3)_9$

## Organic

0.4838  $C_{12}H_8N_2 \cdot H_2O$  0.7724  $C(NH_2)_3Ga(SO_4)_2 \cdot 6H_2O$   
 0.7608  $C(NH_2)_3Al(SO_4)_2 \cdot 6H_2O$

3 m

P3c1  $C_{3v}^3$  No. 158Inorganic - 0  
Organic - 3

## Inorganic

.....

## Organic

0.716  $C_6(OH)_3(NO_2)_3$  1.058  $(C_4H_9)_3P \cdot CuI$   
 0.7874  $C_6H(NO_2)_3(OH)_2$

3 m

P31c  $C_{3v}^4$  No. 159Inorganic - 7  
Organic - 3

## Inorganic

0.3235  $C_3Cr_7$  1.2873  $LiNaSO_4$   
 0.3266  $C_3Mn_7$  1.7392  $AlCu_6(OH)_{12}Cl(SO_4) \cdot 3H_2O$   
 0.7243  $Ge_3N_4$  1.8444  $Ti_6O$   
 0.7250  $N_4S_{13}$

## Organic

0.324  $Cr_7C_3$  0.7446  $[(CH_3)_2N-C_6H_4]_3CCl$   
 0.3266  $Mn_7C_3$



3 m		R3m	$C_{3v}^5$	No. 160	Inorganic - 81 Organic - 28
Inorganic					
0.1784	$SbI_3 \cdot 3S_8$			2.4149	$(Cu, Al)_3 Pb(\theta H)_6(S\theta_4)_2$
0.1821	$AsI_3 \cdot 3S_8$			2.4495	$(Y, Yb, Ca, Zr) P\theta_4 \cdot AlP\theta_4 \cdot 2Al(\theta H)_3$
0.3145	CoS			2.4928	$Al_3 K(\theta H)_6(S\theta_4)_2$
0.3213	CoSe			2.5026	Bi $\theta$
0.3232	NiSe			3.5226	$Ca_3 Si\theta_5$
0.3239	$(Pt(NH_3)_5 Cl)Cl_3 \cdot H_2\theta$			3.5304	$Na_3 BeF_5$
0.3273	NiS			3.5628	$(NH_4)_3( IrCl_6 )NH_4 N\theta_3$
0.3277	NiSe			3.5748	$Ca_3 Si\theta_5$
0.3278	NiS			3.6883	$K_3 Mn\theta_4 Cr\theta_4$
0.4396	$Pb_9 As_4 S_{15}$			4.1799	NaN $\theta$
0.4467	$Li_3 F_3 \theta_9 \cdot 3H_2\theta$			4.2226	NaCN $\theta$
0.4490	$(Na, Ca)(Mg, Fe)_3 B_3 Al_6 Si_6(\theta, \theta H, F)_{31}$			4.5545	$Pb_2 \theta C\theta_3 \cdot 2H_2\theta$
0.4511	$NaMg_3 Al_6 B_3 Si_6 \theta_{27}(\theta H, F)_4$			4.8966	$Cu_5 FeS_4$
0.4511	$(Na, Ca, K)(Mg, Fe)_3(Al, Fe, Ti)_6 B_3 Si_6 \theta_{27}[(\theta H, F)_4]$			5.2839	$CuCrSe_2$
0.4518	$NaMg_3 Al_6 B_3 Si_6 \theta_{27}(\theta H)_4$			5.3453	$Nb_{1+x} S_2$
0.6125	RbN $\theta_3$			5.4032	$CuCrS_2$
0.6229	AlMn			5.4725	$NbSe_2$
0.6240	$Al_8 Cr_5$			5.7563	$AgCrSe_2$
1.0741	$PbTa_2 \theta_6$			5.7975	MoS $_2$
1.1004	$PbNb_2 \theta_6$			5.8041	MoS $_2$
1.2318	$Al_2 Cu_3$			5.8286	MoS $_2$
1.2408	KI $\theta_3$			5.8844	$AgCrS_2$
1.2650	$CsBr\theta_3$			5.8906	MoSe $_2$
1.2848	$CsCl\theta_3$			6.3811	GaSe
1.3019	$NH_4 Br\theta_3$			7.0349	$K_{0.5} CrSe_2$
1.3025	$RbBr\theta_3$			7.1037	$In_2 Se_3$
1.3089	$TlBr\theta_3$			7.3508	ZnS
1.3293	$TlCl\theta_3$			9.8010	ZnS
1.3422	$NH_4 Cl\theta_3$			12.2402	ZnS
1.3424	$RbCl\theta_3$			12.2681	CSi
1.3555	$KBr\theta_3$			17.1518	ZnS
1.6776	KN $\theta_3$			17.1754	CSi
2.2702	$Fe_3 Na(\theta H)_6(S\theta_4)_2$			26.9899	CSi
2.2715	$AgFe_3(\theta H)_6(S\theta_4)_2$			41.7110	CSi
2.3066	$Al_2 Ca_2(P\theta_4)_2(\theta H)_4 \cdot H_2\theta$			46.6296	CSi
2.3124	$Fe_3(\theta H)_5(S\theta_4)_2 \cdot 2H_2\theta$			56.4338	CSi
2.3511	$(Cu, Fe, Al)_3 Pb(\theta H)_6(S\theta_4)_2$			71.1542	CSi
2.3603	$Fe_3(\theta H)_5(S\theta_4)_2 \cdot 2H_2\theta$			73.6192	CSi
2.3611	$NH_4 Fe_3(\theta H)_6(S\theta_4)_2$			85.8967	CSi
2.3611	$Fe_3 K(S\theta_4)_2(\theta H)_6$			115.313	CSi
				321.404	CSi
Organic					
0.1826	$CHI_3 \cdot 3S_8$			4.2450	$C_6 H_{18} \theta_3 Si_3$
0.3818	$Sm(HC\theta)_3 \cdot 0.2H_2\theta$			4.5545	$Pb_2 \theta C\theta_3 \cdot 2H_2\theta$
0.3827	$Nd(HC\theta)_3 \cdot 0.2H_2\theta$			7.2628	$(C_9 H_{17} NH_3)_2 Se\theta_4$
0.3829	$Pr(HC\theta)_3 \cdot 0.2H_2\theta$			12.27	SiC
0.3846	$Ce(HC\theta)_3 \cdot 0.2H_2\theta$			17.175	SiC
0.3882	$C_9 H_{12}$			26.990	SiC
0.632	$(H_3 C)_3 N-BH_3$			41.71	SiC
0.653	$(H_3 C)_3 N-BF_3$			46.6296	SiC
0.6725	$(CH_3)_3 N \cdot Se\theta_3$			56.4338	SiC
0.7131	$(CH_3)_3 N \cdot GaH_3$			71.15	SiC
0.7455	$(CH_2)_6 N_4 \cdot 6H_2\theta$			73.619	SiC
0.7813	$(CH_3)_3 N \cdot B_3 H_7$			85.897	SiC
0.866	ICN			115.31	SiC
4.223	NaCN $\theta$			321.40	SiC

3 m		R3c	$C_{3v}^6$	No. 161	Inorganic - 10 Organic - 26
Inorganic					
0.7888	$Ag_3 SbS_3$			1.2088	$K_3 ThH_4(N\theta_3)_{11}$
0.8049	$Ag_3 AsS_3$			1.3223	$P_4 \theta_{10}$
0.8052	$Ag_3 AsS_3$			2.6921	$LiNb\theta_3$
0.8053	$Ag_3 AsS_3$			2.7757	$LiU\theta_3$
0.8781	AgCN			3.5785	$LiNa_3(S\theta_4)_2 \cdot 6H_2\theta$
Organic					
0.2028	$C_{23} H_{16} BrN\theta$			0.7393	$CH(S\theta_2 CH_3)_3$
0.5964	$C_9 H_{12}(AgN\theta_3)_3$			0.7949	$(CH_3 \theta \theta C)_3 C_3 H_3$

R3c C<sub>3v</sub><sup>6</sup> No. 161 (continued)

## Organic (continued)

0.877	AgCN	3.5560	Mn[OC(NH <sub>2</sub> )NHCH <sub>3</sub> ] <sub>6</sub> S <sub>2</sub> θ <sub>3</sub>
0.8888	C <sub>3</sub> H <sub>6</sub> θ <sub>3</sub>	3.568	Co[OC(NH <sub>2</sub> )NHCH <sub>3</sub> ] <sub>6</sub> S <sub>2</sub> θ <sub>3</sub>
1.0543	H <sub>3</sub> C <sub>3</sub> (CN) <sub>3</sub>	3.569	Zn[OC(NH <sub>2</sub> )NHCH <sub>3</sub> ] <sub>6</sub> S <sub>2</sub> θ <sub>3</sub>
1.179	CH <sub>3</sub> CθNH <sub>2</sub>	3.578	Ni[OC(NH <sub>2</sub> )NHCH <sub>3</sub> ] <sub>6</sub> S <sub>2</sub> θ <sub>3</sub>
1.6221	KFe(NH <sub>2</sub> NHCθθ) <sub>3</sub>	3.673	Cu[OC(NH <sub>2</sub> )NHCH <sub>3</sub> ] <sub>6</sub> S <sub>2</sub> θ <sub>3</sub>
1.6393	KCo(NH <sub>2</sub> NHCθθ) <sub>3</sub>	3.677	Ni[OC(NH <sub>2</sub> )NHCH <sub>3</sub> ] <sub>6</sub> S <sub>2</sub> θ <sub>3</sub>
1.6440	KNi(NH <sub>2</sub> NHCθθ) <sub>3</sub>	3.677	Cd[OC(NH <sub>2</sub> )NHCH <sub>3</sub> ] <sub>6</sub> S <sub>2</sub> θ <sub>3</sub>
1.6488	KZn(N <sub>2</sub> H <sub>3</sub> Cθθ) <sub>3</sub>	3.6819	Zn[OC(NH <sub>2</sub> )NHCH <sub>3</sub> ] <sub>6</sub> S <sub>2</sub> θ <sub>3</sub>
2.5581	C <sub>6</sub> H <sub>12</sub> θ <sub>3</sub> •2NH <sub>3</sub>	3.688	Cd[OC(NH <sub>2</sub> )NHCH <sub>3</sub> ] <sub>6</sub> S <sub>2</sub> θ <sub>3</sub>
2.5789	C <sub>6</sub> H <sub>15</sub> N <sub>3</sub> •2H <sub>2</sub> θ	3.6906	Mn[OC(NH <sub>2</sub> )NHCH <sub>3</sub> ] <sub>6</sub> S <sub>2</sub> θ <sub>3</sub>
2.675	C <sub>6</sub> H <sub>12</sub> θ <sub>3</sub> •2H <sub>2</sub> θ	3.7426	Co[OC(NH <sub>2</sub> )NHCH <sub>3</sub> ] <sub>6</sub> S <sub>2</sub> θ <sub>3</sub>

 $\bar{3} \frac{2}{m}$ P $\bar{3}1m$ D $\frac{1}{3d}$ 

No. 162

Inorganic - 15  
Organic - 3

## Inorganic

0.6097	Ni(H <sub>2</sub> θ) <sub>6</sub> [Sb(θH) <sub>6</sub> ] <sub>2</sub>	0.9402	Ta <sub>6</sub> Cl <sub>14</sub> •7H <sub>2</sub> θ
0.6120	Mg(H <sub>2</sub> θ) <sub>6</sub> [Sb(θH) <sub>6</sub> ] <sub>2</sub>	1.1454	Na <sub>3</sub> (F, Cl)Sθ <sub>4</sub>
0.6162	UTa <sub>2</sub> θ <sub>8</sub>	1.2227	Niθ
0.6262	Cu(NH <sub>3</sub> ) <sub>3</sub> (Sb(θH) <sub>6</sub> ) <sub>2</sub> •3H <sub>2</sub> θ	1.5245	K <sub>2</sub> Pt(SCN) <sub>6</sub>
0.6598	CoI <sub>2</sub> •6H <sub>2</sub> θ	1.5436	(NH <sub>4</sub> ) <sub>2</sub> Pt(SCN) <sub>6</sub>
0.9229	Fe <sub>2</sub> N	1.5511	Rb <sub>2</sub> Pt(SCN) <sub>6</sub>
0.9357	Li <sub>2</sub> ZrF <sub>6</sub>	1.5850	Na <sub>2</sub> Sθ <sub>4</sub> •Na(F, Cl)
0.9372	Al(θH) <sub>3</sub>		

## Organic

1.525	K <sub>2</sub> Pt(SCN) <sub>6</sub>	1.551	Rb <sub>2</sub> Pt(SCN) <sub>6</sub>
1.543	(NH <sub>4</sub> ) <sub>2</sub> Pt(SCN) <sub>6</sub>		

 $\bar{3} \frac{2}{m}$ P $\bar{3}1c$ D $\frac{2}{3d}$ 

No. 163

Inorganic - 12  
Organic - 4

## Inorganic

0.6153	Sn <sub>5</sub> Ti <sub>6</sub>	1.8544	Ti <sub>3</sub> θ
1.0420	PhAs <sub>2</sub> S <sub>4</sub>	1.8845	Cr <sub>2</sub> S <sub>3</sub>
1.5588	Cr <sub>1-x</sub> Te	1.9093	NaSbF <sub>4</sub> (θH) <sub>2</sub>
1.5606	Fe <sub>2</sub> (Sθ <sub>4</sub> ) <sub>3</sub> •9H <sub>2</sub> θ	1.9239	Cr <sub>5</sub> S <sub>6</sub>
1.7552	Tl <sub>2</sub> Cl <sub>3</sub>	2.3772	KAg(CN) <sub>2</sub>
1.7717	Cr <sub>2</sub> Ie <sub>3</sub>	3.7370	N <sub>2</sub> W <sub>2.2</sub>

## Organic

1.0738	Cu(NH <sub>2</sub> •CH <sub>2</sub> CH <sub>2</sub> •NH <sub>2</sub> ) <sub>3</sub> Sθ <sub>4</sub>	1.2751	MgNa[Cr(C <sub>2</sub> θ <sub>4</sub> ) <sub>3</sub> ]•8H <sub>2</sub> θ
1.248	KI•KI <sub>3</sub> •6(CH <sub>3</sub> CθNHCH <sub>3</sub> )	2.377	KAg(CN) <sub>2</sub>

 $\bar{3} \frac{2}{m}$ P $\bar{3}m1$ D $\frac{3}{3d}$ 

No. 164

Inorganic - 225  
Organic - 9

## Inorganic

0.5356	(Fe, Mn) <sub>8</sub> Si <sub>6</sub> θ <sub>15</sub> (θH, Cl) <sub>10</sub>	0.8026	Cs <sub>2</sub> RuF <sub>6</sub>
0.5359	(Mn, Fe) <sub>8</sub> Si <sub>6</sub> θ <sub>15</sub> (θH, Cl) <sub>10</sub>	0.8055	Cs <sub>2</sub> PtF <sub>6</sub>
0.5507	UCl <sub>6</sub>	0.8056	K <sub>2</sub> PtF <sub>6</sub>
0.5576	Na <sub>2</sub> TiF <sub>6</sub>	0.8056	K <sub>2</sub> RuF <sub>6</sub>
0.5716	Na <sub>2</sub> SiF <sub>6</sub>	0.8059	Cs <sub>2</sub> UCl <sub>6</sub>
0.6123	Cr <sub>x</sub> Ti	0.8065	Cs <sub>2</sub> TiF <sub>6</sub>
0.7174	Cd <sub>2</sub> Y	0.8078	Cs <sub>2</sub> CeCl <sub>6</sub>
0.7816	Cs <sub>2</sub> ZrF <sub>6</sub>	0.8081	Cs <sub>2</sub> RhF <sub>6</sub>
0.7825	Rb <sub>2</sub> ZrF <sub>6</sub>	0.8087	(NH <sub>4</sub> ) <sub>2</sub> TiF <sub>6</sub>
0.7825	Cs <sub>2</sub> HfF <sub>6</sub>	0.8101	K <sub>2</sub> RhF <sub>6</sub>
0.7850	Rb <sub>2</sub> HfF <sub>6</sub>	0.8104	Rb <sub>2</sub> PtF <sub>6</sub>
0.7855	K <sub>2</sub> ReF <sub>6</sub>	0.8116	Cs <sub>2</sub> PuCl <sub>6</sub>
0.7863	K <sub>2</sub> ReF <sub>6</sub>	0.8129	Rb <sub>2</sub> TiF <sub>6</sub>
0.7871	(NH <sub>4</sub> ) <sub>2</sub> ReF <sub>6</sub>	0.8139	Rb <sub>2</sub> RhF <sub>6</sub>
0.7910	Rb <sub>2</sub> ReF <sub>6</sub>	0.8144	K <sub>2</sub> MnF <sub>6</sub>
0.7921	Cs <sub>2</sub> ReF <sub>6</sub>	0.8147	K <sub>2</sub> TiF <sub>6</sub>
0.7930	Cs <sub>2</sub> ThCl <sub>6</sub>	0.8162	(NH <sub>4</sub> ) <sub>2</sub> GeF <sub>6</sub>
0.7999	K <sub>2</sub> (TcF <sub>6</sub> )	0.8176	Tl <sub>2</sub> TiF <sub>6</sub>
0.8015	Rb <sub>2</sub> (TcF <sub>6</sub> )	0.8230	Rb <sub>2</sub> GeF <sub>6</sub>

P $\bar{3}$ m1 D $\bar{3}$ d No. 164 (continued)

## Inorganic (continued)

0.8274	K <sub>2</sub> GeF <sub>6</sub>	1.5606	Cr <sub>5</sub> Te <sub>6</sub>
0.8292	(NH <sub>4</sub> ) <sub>2</sub> SiF <sub>6</sub>	1.5619	Ce <sub>2</sub> Te <sub>3</sub>
0.8378	AlBr <sub>3</sub> SH <sub>2</sub>	1.5643	Am <sub>2</sub> Te <sub>3</sub>
0.8505	AgTlSe <sub>2</sub>	1.5651	Nd <sub>2</sub> Te <sub>3</sub>
0.9150	CaSe <sub>4</sub> •0.5H <sub>2</sub> O	1.5660	Pm <sub>2</sub> Te <sub>3</sub>
0.9451	CaSe <sub>4</sub> •0.5H <sub>2</sub> O	1.5678	SiTe <sub>2</sub>
0.9744	MoN	1.5781	CW <sub>2</sub>
0.9790	MoN	1.5790	N <sub>3</sub> U <sub>2</sub>
1.0497	U <sub>3</sub>	1.5808	Mg <sub>3</sub> Sb <sub>2</sub>
1.2061	Ga <sub>3</sub> Ni <sub>2</sub>	1.5809	CMo <sub>2</sub>
1.2070	In <sub>3</sub> Ni <sub>2</sub>	1.5822	As <sub>2</sub> Mg <sub>3</sub>
1.2135	Al <sub>3</sub> Ni <sub>2</sub>	1.5862	Bi <sub>2</sub> Mg <sub>3</sub>
1.2225	Cs <sub>3</sub> Fe <sub>2</sub> Cl <sub>9</sub>	1.5874	ZrS <sub>2</sub>
1.2247	Cs <sub>3</sub> Sb <sub>2</sub> Cl <sub>9</sub>	1.5891	As <sub>2</sub> Mg <sub>2</sub> Mn
1.2248	Al <sub>3</sub> Pd <sub>2</sub>	1.5897	ZrS <sub>2</sub>
1.2251	Ga <sub>3</sub> Pt <sub>2</sub>	1.5913	CTa <sub>2</sub>
1.2291	Al <sub>3</sub> Pt <sub>2</sub>	1.5932	Th <sub>2</sub> N <sub>2</sub> O
1.2332	Al <sub>3</sub> Tc <sub>2</sub>	1.5949	Fe <sub>2</sub> N
1.2381	Ca <sub>2</sub> Si <sub>4</sub>	1.6000	ZrS <sub>2</sub>
1.2467	Au <sub>3</sub> In <sub>2</sub>	1.6007	Zn(OH) <sub>2</sub>
1.2502	Fe <sub>1.67</sub> Ge	1.6058	HfS <sub>2</sub>
1.2700	PdTe <sub>2</sub>	1.6084	Ag <sub>2</sub> O
1.2903	K <sub>3</sub> Na(S <sub>4</sub> ) <sub>2</sub>	1.6109	Zn(OH) <sub>1.5</sub> Fe <sub>0.5</sub>
1.2940	(K,NH <sub>4</sub> ) <sub>3</sub> Na(S <sub>4</sub> ) <sub>2</sub>	1.6120	CdI <sub>2</sub>
1.2968	PtTe <sub>2</sub>	1.6160	SnS <sub>2</sub>
1.3207	Na <sub>2</sub> BeF <sub>4</sub>	1.6199	MnBr <sub>2</sub>
1.3293	Tl <sub>2</sub> S <sub>4</sub>	1.6220	ZrCl <sub>3</sub>
1.3461	CaNaP <sub>4</sub>	1.6226	(Mg <sub>0.62</sub> Zn <sub>0.38</sub> ) <sub>3</sub> Sb <sub>2</sub>
1.3482	Na <sub>2</sub> S <sub>4</sub>	1.6279	ZrSe <sub>2</sub>
1.3573	Cd(OH) <sub>2</sub>	1.6306	ZrSe <sub>2</sub>
1.3620	CaKP <sub>4</sub>	1.6373	Ti <sub>2</sub> O
1.3631	PtSe <sub>2</sub>	1.6394	MnI <sub>2</sub>
1.3633	CaNaP <sub>4</sub>	1.6398	MgBr <sub>2</sub>
1.3691	(Cd,Mn)(OH) <sub>2</sub>	1.6401	VBr <sub>2</sub>
1.3692	Ca(OH) <sub>2</sub>	1.6402	FeBr <sub>2</sub>
1.3701	K <sub>2</sub> S <sub>4</sub>	1.6433	HfSe <sub>2</sub>
1.3703	NiTe <sub>2</sub>	1.6441	GeI <sub>2</sub>
1.3719	NiTe <sub>2</sub>	1.6469	Mn <sub>2</sub> (OH) <sub>3</sub> Cl
1.3723	IrTe <sub>2</sub>	1.6498	TiCl <sub>2</sub>
1.3765	Rb <sub>2</sub> S <sub>4</sub>	1.6594	TiI <sub>2</sub>
1.3794	NiTeSe	1.6608	CoBr <sub>2</sub>
1.3796	Fe(OH) <sub>2</sub>	1.6618	MgI <sub>2</sub>
1.3800	(Ca,Cd)(OH) <sub>2</sub>	1.6627	Fe <sub>2</sub> (OH) <sub>3</sub> Cl
1.3801	RhTe <sub>2</sub>	1.6630	CoBr <sub>2</sub>
1.4012	Mn(OH) <sub>2</sub>	1.6637	Cr <sub>7</sub> S <sub>8</sub>
1.4222	PtS <sub>2</sub>	1.6675	VI <sub>2</sub>
1.4249	CdCl <sub>0.26</sub> (OH) <sub>1.74</sub>	1.6708	FeI <sub>2</sub>
1.4250	Mn(OH) <sub>2</sub>	1.6728	TiS <sub>2</sub>
1.4279	CoTe <sub>2</sub>	1.6753	TiS <sub>2</sub>
1.4295	Ni(OH) <sub>2</sub>	1.6785	ZrTe <sub>2</sub>
1.4585	Co(OH) <sub>2</sub>	1.6793	CoI <sub>2</sub>
1.4623	Co(OH) <sub>2</sub>	1.6814	TiS <sub>2</sub>
1.4736	Ni <sub>0.8</sub> Zn <sub>0.2</sub> (OH) <sub>2</sub>	1.6852	ZrTe <sub>2</sub>
1.4742	Ni(OH) <sub>2</sub>	1.6905	TiSe <sub>2</sub>
1.4792	(Co,Ni)(OH) <sub>2</sub>	1.6969	TiSe <sub>2</sub>
1.4794	(Co,Mg)(OH) <sub>2</sub>	1.6984	TiSe <sub>2</sub>
1.4794	(Co,Zn)(OH) <sub>2</sub>	1.7050	Ce <sub>2</sub> Te <sub>2</sub> S
1.4992	Ni(OH) <sub>2</sub>	1.7139	La <sub>2</sub> Te <sub>2</sub> S
1.5113	(Ni,Mg)(OH) <sub>2</sub>	1.7175	Pr <sub>2</sub> Te <sub>2</sub> S
1.5115	PbI <sub>2</sub>	1.7181	Ce <sub>2</sub> Te <sub>2</sub> S
1.5197	(Ni,Zn)(OH) <sub>2</sub>	1.7207	Nd <sub>2</sub> Te <sub>2</sub> S
1.5206	Mg(OH) <sub>2</sub>	1.7234	TiTe <sub>2</sub>
1.5296	BiTeBr	1.7237	Pu <sub>2</sub> Te <sub>2</sub> S
1.5298	PbI <sub>2</sub>	1.7252	Sm <sub>2</sub> Te <sub>2</sub> S
1.5315	PbI <sub>2</sub>	1.7267	Co <sub>2</sub> (OH) <sub>3</sub> Cl
1.5388	ZnI <sub>2</sub>	1.7268	Eu <sub>2</sub> Te <sub>2</sub> S
1.5405	(Mg,Zn)(OH) <sub>2</sub>	1.7273	Ni <sub>2</sub> (OH) <sub>3</sub> Cl
1.5414	TmI <sub>2</sub>	1.7311	Gd <sub>2</sub> Te <sub>2</sub> S
1.5441	Ac <sub>2</sub> Te <sub>3</sub>	1.7323	Tb <sub>2</sub> Te <sub>2</sub> S
1.5475	CdCl <sub>0.68</sub> (OH) <sub>1.32</sub>	1.7333	TiTe <sub>2</sub>
1.5536	CaI <sub>2</sub>	1.7363	Dy <sub>2</sub> Te <sub>2</sub> S
1.5536	YbI <sub>2</sub>	1.7400	Ho <sub>2</sub> Te <sub>2</sub> S
1.5573	La <sub>2</sub> Te <sub>3</sub>	1.7400	Y <sub>2</sub> Te <sub>2</sub> S
1.5584	Pr <sub>2</sub> Te <sub>3</sub>	1.7425	Er <sub>2</sub> Te <sub>2</sub> S

P $\bar{3}$ m1 D $\frac{3}{3d}$  No. 164 (continued)

## Inorganic (continued)

1.7449	Tm $\theta_2$ S	1.7841	Lu $\theta_2$ Se
1.7466	Yb $\theta_2$ S	1.8132	CdI $_{0.5}(\theta H)_{1.5}$
1.7486	Lu $\theta_2$ S	1.8191	Nb $\theta_3$ Cl $\theta$
1.7507	Ce $\theta_2$ Se	1.8995	Ag $\theta_2$ F
1.7513	Ta $\theta_2$ S	2.0294	Ba $\theta_5$ Ta $\theta_4$ Se $\theta_{15}$
1.7540	Pr $\theta_2$ Se	2.1935	Co $\theta_2(\theta H)_3(N\theta_3)$
1.7574	Nd $\theta_2$ Se	2.4489	AlCl $\theta_3$
1.7615	Sm $\theta_2$ Se	2.4494	Zr $\theta_3$ P $\theta_2$
1.7640	Eu $\theta_2$ Se	2.4526	Ti $\theta_3$ P $\theta_2$
1.7656	Mg $\theta_2(\theta H)_3$ Cl	2.4590	Al $\theta_3$ Pt $\theta_2$
1.7664	Gd $\theta_2$ Se	3.5649	[Na $\theta_4$ (Ca, Mg) $\theta_2$ Cl $\theta_{12}$ ][Mg $\theta_7$ Al $\theta_4$ ( $\theta H$ ) $\theta_{22}$ ]
1.7691	Tb $\theta_2$ Se	3.8910	Pb $\theta_2$ Bi $\theta_2$ Se $\theta_5$
1.7692	MgCl $_{0.5}(\theta H)_{1.5}$	3.9111	PbBi $\theta_4$ Te $\theta_7$
1.7710	Dy $\theta_2$ Se	4.6830	AgBiS $\theta_2$
1.7743	Ho $\theta_2$ Se	4.7057	AgBiSe $\theta_2$
1.7754	Y $\theta_2$ Se	4.7116	Ag $\theta_2$ Bi $\theta_2$ S $\theta_4$
1.7768	Er $\theta_2$ Se	16.1486	PbBi $\theta_4$ Te $\theta_7$
1.7784	TiCl $\theta_2$	24.1667	PbBi $\theta_4$ Te $\theta_7$
1.7792	Tm $\theta_2$ Se	31.1395	Ba $\theta_{12}(\text{Mn, Zn})_{11}$ Fe $\theta_{78}$ Se $\theta_{140}$
1.7825	Yb $\theta_2$ Se		

## Organic

0.5076	Fe(CNCH $\theta_3$ ) $\theta_6$ Cl $\theta_2$ •3H $\theta_2$ Se	1.5781	W $\theta_2$ C
0.6779	CaC(C[CN] $\theta_2$ ) $\theta_3$ •6H $\theta_2$ Se	1.5809	Mo $\theta_2$ C
0.6799	Ba[C(C[CN] $\theta_2$ ) $\theta_3$ ]•6H $\theta_2$ Se	1.5913	Ta $\theta_2$ C
1.161	(NH $\theta_3$ C $\theta_2$ H $\theta_5$ ) $\theta_2$ SnCl $\theta_6$	7.1429	C $\theta_{12}$ H $\theta_{25}$ SeH
1.196	(NH $\theta_3$ C $\theta_2$ H $\theta_5$ ) $\theta_2$ PtCl $\theta_6$		

P $\bar{3}$ mP $\bar{3}$ c1 D $\frac{4}{3d}$  No. 165Inorganic - 59  
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## Inorganic

1.0092	Cu $\theta_3$ P	1.0258	SrUF $\theta_6$
1.0144	BaThF $\theta_6$	1.0263	Li $\theta_3$ P
1.0146	PbUF $\theta_6$	1.0266	HgMg $\theta_3$
1.0184	PbThF $\theta_6$	1.0276	NpH $\theta_3$
1.0186	CmF $\theta_3$	1.0276	AsLi $\theta_3$
1.0189	AcF $\theta_3$	1.0291	CaThF $\theta_6$
1.0192	AsNa $\theta_3$	1.0321	PuH $\theta_3$
1.0198	Na $\theta_3$ P	1.0348	SmH $\theta_3$
1.0203	AsCu $\theta_3$	1.0355	Bi $\theta_{0.1}$ F $\theta_{2.8}$
1.0205	Li $\theta_3$ Sb	1.0387	GdH $\theta_3$
1.0207	AsK $\theta_3$	1.0389	TbH $\theta_3$
1.0217	BiK $\theta_3$	1.0399	HoH $\theta_3$
1.0219	LaF $\theta_3$	1.0403	DyH $\theta_3$
1.0222	PrF $\theta_3$	1.0405	ErH $\theta_3$
1.0222	NpF $\theta_3$	1.0409	TmH $\theta_3$
1.0224	CeF $\theta_3$	1.0421	Th $\theta_3$ F $\theta_2$
1.0227	PuF $\theta_3$	1.0444	IrMg $\theta_3$
1.0231	UF $\theta_3$	1.0454	LuH $\theta_3$
1.0231	LaF $\theta_3$	1.0470	YH $\theta_3$
1.0232	BiNa $\theta_3$	1.0497	Mg $\theta_3$ Pt
1.0237	AsCu $\theta_3$	1.0518	Na $\theta_3$ V $\theta_4$ •12H $\theta_2$ Se
1.0238	Na $\theta_3$ Sb	1.0522	AuMg $\theta_3$
1.0242	TmF $\theta_3$	1.0526	Mg $\theta_3$ Pd
1.0244	SmF $\theta_3$	1.0532	Na $\theta_3$ P $\theta_4$ •12H $\theta_2$ Se
1.0246	K $\theta_3$ Sb	1.8355	Ca $\theta_2$ (Si, Re, Ti, Al, Sn, Tl) $\theta_3$ (As $\theta_3$ ) $\theta_5$
1.0250	AmF $\theta_3$	2.6841	Mn $\theta_4$ Nb $\theta_2$ Se $\theta_9$
1.0253	AsCu $\theta_3$	2.7367	Co $\theta_4$ Nb $\theta_2$ Se $\theta_9$
1.0255	Cu $\theta_3$ P	3.2178	K $\theta_3$ Rh(SCN) $\theta_6$
1.0256	SrThF $\theta_6$	5.2667	Ca $\theta_4$ Fe $\theta_{14}$ Se $\theta_{25}$
1.0257	AmF $\theta_3$		

## Organic

0.8864	(C $\theta_6$ H $\theta_5$ ) $\theta_6$ P $\theta_6$	1.359	Rh(NH $\theta_2$ •CH $\theta_2$ ) $\theta_6$ Cl $\theta_3$ •3H $\theta_2$ Se
0.9086	(C $\theta_{10}$ H $\theta_8$ N $\theta_2$ ) $\theta_3$ Tl	1.3736	Cr(NH $\theta_2$ •CH $\theta_2$ ) $\theta_6$ Br $\theta_3$ •3H $\theta_2$ Se
0.9167	(C $\theta_{10}$ H $\theta_8$ N $\theta_2$ ) $\theta_3$ V	1.3787	Co(NH $\theta_2$ •CH $\theta_2$ ) $\theta_6$ Br $\theta_3$ •3H $\theta_2$ Se
0.9378	(C $\theta_{10}$ H $\theta_8$ N $\theta_2$ ) $\theta_3$ Cr	1.4897	K(NH $\theta_2$ CH $\theta_2$ CH $\theta_2$ NH $\theta_2$ ) $\theta_3$ Ni(SeCN) $\theta_3$
1.3496	[Co(C $\theta_2$ H $\theta_4$ (NH $\theta_2$ ) $\theta_2$ ) $\theta_3$ ]Cl $\theta_3$ •3H $\theta_2$ Se	3.2178	K $\theta_3$ Rh(SCN) $\theta_6$
1.3509	Cr(NH $\theta_2$ •CH $\theta_2$ ) $\theta_6$ Cl $\theta_3$ •3H $\theta_2$ Se		

$\bar{3} \frac{2}{m}$	$R\bar{3}m$	$D_{3d}^5$	No. 166	Inorganic - 451 Organic - 18
Inorganic				
0.5074	FeF <sub>2</sub> •4H <sub>2</sub> O		1.4574	Co <sub>17</sub> Sm <sub>2</sub>
0.6537	PtCl <sub>2</sub>		1.4580	Co <sub>17</sub> Nd <sub>2</sub>
0.7274	Mo <sub>6</sub> (OH) <sub>4</sub> Cl <sub>8</sub> •14H <sub>2</sub> O		1.4582	Co <sub>17</sub> Y <sub>2</sub>
0.7770	(NH <sub>4</sub> ) <sub>6</sub> MnMo <sub>9</sub> O <sub>32</sub> •6H <sub>2</sub> O		1.4582	Co <sub>17</sub> Tb <sub>2</sub>
0.7770	(NH <sub>4</sub> ) <sub>6</sub> NiMo <sub>9</sub> O <sub>32</sub> •6H <sub>2</sub> O		1.4584	Ce <sub>2</sub> Co <sub>17</sub>
0.9625	BaPdF <sub>6</sub>		1.4585	Be <sub>17</sub> Hf <sub>2</sub>
0.9647	BaMnF <sub>6</sub>		1.4593	Fe <sub>17</sub> Gd <sub>2</sub>
0.9681	Po		1.4594	Co <sub>17</sub> Dy <sub>2</sub>
0.9687	SrPdF <sub>6</sub>		1.4597	Be <sub>17</sub> Ti <sub>2</sub>
0.9687	BaTiF <sub>6</sub>		1.4609	Co <sub>17</sub> Tb <sub>2</sub>
0.9729	NbS		1.4609	Co <sub>17</sub> Y <sub>2</sub>
0.9743	BaGeF <sub>6</sub>		1.4618	Th <sub>2</sub> Zn <sub>17</sub>
0.9758	BaSiF <sub>6</sub>		1.4622	Y <sub>2</sub> Zn <sub>17</sub>
0.9758	BaRuF <sub>6</sub>		1.4622	Ba <sub>2</sub> Mg <sub>17</sub>
0.9810	SrPtF <sub>6</sub>		1.4629	Fe <sub>17</sub> Tb <sub>2</sub>
0.9810	BaIrF <sub>6</sub>		1.4631	Be <sub>17</sub> Nb <sub>2</sub>
0.9811	BaPtF <sub>6</sub>		1.4638	Ho <sub>2</sub> Zn <sub>17</sub>
0.9920	KRuF <sub>6</sub>		1.4649	Be <sub>17</sub> Ti <sub>2</sub>
0.9979	BaReF <sub>6</sub>		1.4652	Ce <sub>2</sub> Fe <sub>17</sub>
1.0000	BaSnF <sub>6</sub>		1.4665	Er <sub>2</sub> Zn <sub>17</sub>
1.0025	RbAsF <sub>6</sub>		1.4669	Fe <sub>17</sub> Y <sub>2</sub>
1.0028	FeSiF <sub>6</sub> •6H <sub>2</sub> O		1.7315	NaN <sub>3</sub>
1.0056	RbVF <sub>6</sub>		1.7948	KN <sub>3</sub>
1.0056	RbRuF <sub>6</sub>		1.8124	KN <sub>3</sub>
1.0088	CsSbF <sub>6</sub>		1.8126	HCl•H <sub>2</sub> O
1.0094	BaPbF <sub>6</sub>		1.8249	Na <sub>3</sub> Co(N <sub>3</sub> ) <sub>6</sub>
1.0107	CsNbF <sub>6</sub>		1.8435	TaTe
1.0148	RbReF <sub>6</sub>		1.8451	NbTe
1.0210	NH <sub>4</sub> SbF <sub>6</sub>		1.9288	CsICl <sub>2</sub>
1.0210	RbSbF <sub>6</sub>		1.9365	Hg
1.0236	RbTaF <sub>6</sub>		1.9423	RbSeH
1.0251	RbNbF <sub>6</sub>		1.9570	K <sub>2</sub> Sn(OH) <sub>6</sub>
1.0261	CsTaF <sub>6</sub>		1.9721	Re <sub>3</sub> Cl <sub>9</sub>
1.0271	Cu <sub>2</sub> (OH) <sub>3</sub> Cl		1.9814	B <sub>13</sub> P <sub>2</sub>
1.0302	CsVF <sub>6</sub>		1.9899	KSeH
1.0302	CsIrF <sub>6</sub>		1.9977	RbSH
1.0333	NH <sub>4</sub> NbF <sub>6</sub>		2.0020	KSH
1.0344	NH <sub>4</sub> TaF <sub>6</sub>		2.0119	B <sub>4</sub> Si
1.0345	CsRuF <sub>6</sub>		2.0446	KN <sub>3</sub>
1.0364	CsAsF <sub>6</sub>		2.0460	NaSeH
1.0366	TlSbF <sub>6</sub>		2.0516	NaSH
1.0395	CsReF <sub>6</sub>		2.1032	Co <sub>2</sub> (OH) <sub>3</sub> Br
1.0793	CaAl <sub>2</sub> (Si <sub>3</sub> ) <sub>4</sub> •6H <sub>2</sub> O		2.1069	(Na, Ca, Fe) <sub>6</sub> ZrSi <sub>6</sub> Si <sub>18</sub> (OH, Cl)
1.0853	Ca <sub>2-x</sub> Na <sub>x</sub> Al <sub>4-x</sub> Si <sub>8+x</sub> •24•10H <sub>2</sub> O		2.1159	Co <sub>2</sub> (OH) <sub>3</sub> Cl
1.0873	CaAl <sub>2</sub> (Si <sub>3</sub> ) <sub>4</sub> •6H <sub>2</sub> O		2.1159	Fe <sub>2</sub> (OH) <sub>3</sub> Cl
1.0891	CaAl <sub>2</sub> (Si <sub>3</sub> ) <sub>4</sub> •6H <sub>2</sub> O		2.1643	B <sub>4</sub> C
1.0944	Na <sub>4</sub> Al <sub>4</sub> Si <sub>8</sub> •24•12H <sub>2</sub> O		2.1665	B
1.1606	CaAl <sub>2</sub> (Si <sub>3</sub> ) <sub>4</sub>		2.3340	(Bi, Ca)Al <sub>3</sub> (P <sub>3</sub> , Si <sub>3</sub> ) <sub>2</sub> (OH) <sub>6</sub>
1.2178	PrCo <sub>3</sub>		2.3472	Fe <sub>3</sub> K(OH) <sub>6</sub> (Cr <sub>3</sub> ) <sub>2</sub>
1.2408	LiPb		2.3521	Al <sub>3</sub> Ca(OH) <sub>6</sub> (P <sub>3</sub> )(S <sub>3</sub> )
1.2426	BiFe <sub>3</sub>		2.3552	Cr <sub>3</sub> H(S <sub>3</sub> ) <sub>2</sub> (OH) <sub>6</sub>
1.2450	Zr <sub>3</sub> Se <sub>4</sub>		2.3555	Al <sub>3</sub> (Ce, Sr)(OH) <sub>6</sub> (P <sub>3</sub> ) <sub>2</sub>
1.2536	TlI <sub>3</sub>		2.3632	Al <sub>3</sub> Ba(OH) <sub>5</sub> (P <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> O
1.3245	Na <sub>2</sub> CaU <sub>2</sub> (C <sub>3</sub> ) <sub>3</sub> •6H <sub>2</sub> O		2.3689	Al <sub>3</sub> (Sr, Ce)(OH) <sub>5</sub> (P <sub>3</sub> ) <sub>2</sub> •H <sub>2</sub> O
1.3439	CsCN		2.3807	Al <sub>2</sub> •4Zn
1.4503	Fe <sub>17</sub> Gd <sub>2</sub>		2.3914	Ga <sub>3</sub> (H <sub>3</sub> )(OH) <sub>6</sub> (S <sub>3</sub> ) <sub>2</sub>
1.4506	Fe <sub>7</sub> Pr		2.4047	LaNi <sub>3</sub>
1.4514	Fe <sub>7</sub> Nd		2.4093	LaCo <sub>3</sub>
1.4517	Fe <sub>17</sub> Nd <sub>2</sub>		2.4138	Al <sub>3</sub> Sr(OH) <sub>6</sub> (S <sub>3</sub> )(P <sub>3</sub> )
1.4525	Co <sub>17</sub> Dy <sub>2</sub>		2.4265	NdAl <sub>3</sub>
1.4527	Fe <sub>7</sub> Sm		2.4265	LaGa <sub>3</sub>
1.4534	Fe <sub>17</sub> Pr <sub>2</sub>		2.4311	PrAl <sub>3</sub>
1.4535	Co <sub>17</sub> Pr <sub>2</sub>		2.4320	SmAl <sub>3</sub>
1.4541	Co <sub>17</sub> Nd <sub>2</sub>		2.4333	TlTe
1.4554	Co <sub>17</sub> Pr <sub>2</sub>		2.4440	LaAl <sub>3</sub>
1.4555	Fe <sub>17</sub> Tb <sub>2</sub>		2.4495	Ni <sub>3</sub> Pb <sub>2</sub> S <sub>2</sub>
1.4555	Al <sub>10.5</sub> Ce <sub>2</sub> Cu <sub>6.5</sub>		2.4769	ThSiW <sub>12</sub> •40•30H <sub>2</sub> O
1.4557	Fe <sub>7</sub> Gd		2.4778	Al <sub>3</sub> K(OH) <sub>6</sub> (S <sub>3</sub> ) <sub>2</sub>
1.4561	Co <sub>17</sub> Gd <sub>2</sub>		2.4923	ThSiW <sub>12</sub> •40•27H <sub>2</sub> O
1.4567	Co <sub>17</sub> Sm <sub>2</sub>		2.5000	Li <sub>3</sub> HSiW <sub>12</sub> •40•24H <sub>2</sub> O
1.4568	Ce <sub>2</sub> Co <sub>17</sub>		2.5032	Al <sub>3</sub> K(OH) <sub>6</sub> (S <sub>3</sub> ) <sub>2</sub>
1.4569	Be <sub>17</sub> Zr <sub>2</sub>		2.5500	H <sub>3</sub> PW <sub>12</sub> •40•24H <sub>2</sub> O
1.4569	Al <sub>10</sub> Ce <sub>2</sub> Mn <sub>7</sub>		2.5513	FeHSiW <sub>12</sub> •40•24H <sub>2</sub> O
1.4573	Al <sub>2</sub> Ce <sub>2</sub> Co <sub>15</sub>		2.5605	B

R $\bar{3}m$  D $\bar{5}$ <sub>3d</sub> No. 166 (continued)

## Inorganic

2.6094	Bi	4.4968	Nf <sub>4</sub> Pu $\bar{2}$ F <sub>2</sub>
2.6169	Sb	4.4981	RbAm $\bar{2}$ F <sub>2</sub>
2.6346	Zn <sub>2</sub> SiW <sub>12</sub> $\bar{4}$ <sub>0</sub> •27H <sub>2</sub> $\bar{6}$	4.4999	KAm $\bar{2}$ F <sub>2</sub>
2.6355	Cu <sub>2</sub> SiW <sub>12</sub> $\bar{4}$ <sub>0</sub> •27H <sub>2</sub> $\bar{6}$	4.5149	CdU $\bar{4}$
2.6414	Li <sub>3</sub> HSiW <sub>12</sub> $\bar{4}$ <sub>0</sub> •26H <sub>2</sub> $\bar{6}$	4.5191	Na <sub>2</sub> U $\bar{2}$ $\bar{6}$ <sub>7</sub>
2.6460	Cd <sub>3</sub> (PW <sub>12</sub> $\bar{4}$ <sub>0</sub> ) <sub>2</sub> •48H <sub>2</sub> $\bar{6}$	4.5256	DCr $\bar{2}$
2.6503	Ca <sub>2</sub> SiW <sub>12</sub> $\bar{4}$ <sub>0</sub> •26H <sub>2</sub> $\bar{6}$	4.5296	CdCl <sub>2</sub>
2.6503	Mn <sub>3</sub> (PW <sub>12</sub> $\bar{4}$ <sub>0</sub> ) <sub>2</sub> •48H <sub>2</sub> $\bar{6}$	4.5309	Ca(U $\bar{6}$ ) $\bar{6}$ <sub>2</sub>
2.6513	FeHSiW <sub>12</sub> $\bar{4}$ <sub>0</sub> •28H <sub>2</sub> $\bar{6}$	4.5453	CdCl <sub>2</sub>
2.6521	CrHSiW <sub>12</sub> $\bar{4}$ <sub>0</sub> •28H <sub>2</sub> $\bar{6}$	4.5595	PbI <sub>2</sub>
2.6531	Co <sub>3</sub> (PW <sub>12</sub> $\bar{4}$ <sub>0</sub> ) <sub>2</sub> •48H <sub>2</sub> $\bar{6}$	4.5791	CaNp $\bar{4}$
2.6557	Ni <sub>3</sub> (PW <sub>12</sub> $\bar{4}$ <sub>0</sub> ) <sub>2</sub> •48H <sub>2</sub> $\bar{6}$	4.5791	SrPu $\bar{4}$
2.6575	AlHSiW <sub>12</sub> $\bar{4}$ <sub>0</sub> •28H <sub>2</sub> $\bar{6}$	4.5865	Sr(U $\bar{6}$ ) $\bar{6}$ <sub>2</sub>
2.6753	Ca <sub>2</sub> (SiMo <sub>12</sub> $\bar{4}$ <sub>0</sub> )•24H <sub>2</sub> $\bar{6}$	4.5900	SrU $\bar{3}$ .58
2.6822	Ba <sub>2</sub> SiW <sub>12</sub> $\bar{4}$ <sub>0</sub> •24H <sub>2</sub> $\bar{6}$	4.6152	Be <sub>3</sub> Nb
2.6884	Ba <sub>3</sub> (PW <sub>12</sub> $\bar{4}$ <sub>0</sub> ) <sub>2</sub> •48H <sub>2</sub> $\bar{6}$	4.6247	Be <sub>3</sub> Ta
2.7100	AsSb	4.6491	Co $\bar{6}$ (OH)
2.8057	As	4.6667	Pb(Fe <sub>3</sub> (S $\bar{4}$ ) <sub>2</sub> (OH) <sub>6</sub> ) <sub>2</sub>
3.2438	N <sub>2</sub> H <sub>6</sub> F <sub>2</sub>	4.7159	(Ba <sub>0.95</sub> Ca <sub>0.05</sub> )Pb <sub>3</sub>
3.4037	$\bar{6}$ <sub>2</sub>	4.7215	ZnCl <sub>2</sub>
3.4127	Al <sub>3</sub> Y	4.7275	AgBiSe <sub>2</sub>
3.4218	Al <sub>3</sub> Tb	4.7280	CdBr <sub>2</sub>
3.4281	Pb <sub>3</sub> (V $\bar{4}$ ) <sub>2</sub>	4.7351	LiRb $\bar{6}$
3.4300	Al <sub>3</sub> Tb	4.7400	MnCl <sub>2</sub>
3.5364	BaPb <sub>3</sub>	4.7483	Be <sub>3</sub> Ti
3.5800	Sr <sub>3</sub> (As $\bar{4}$ ) <sub>2</sub>	4.7506	AgBiTe <sub>2</sub>
3.5830	Sr <sub>3</sub> (V $\bar{4}$ ) <sub>2</sub>	4.7779	ZnBr <sub>2</sub>
3.6213	Sr <sub>3</sub> (Cr $\bar{4}$ ) <sub>2</sub>	4.7815	NaLaSe <sub>2</sub>
3.6299	CaCN <sub>2</sub>	4.7922	LiHoS <sub>2</sub>
3.6653	(Co <sub>0.67</sub> Ni <sub>0.33</sub> ) <sub>3</sub> V	4.8077	LiErS <sub>2</sub>
3.6742	Sr <sub>3</sub> (P $\bar{4}$ ) <sub>2</sub>	4.8173	P
3.6772	Ni <sub>3</sub> (Ti <sub>0.89</sub> Nb <sub>0.11</sub> )	4.8245	NaCeSe <sub>2</sub>
3.6816	Ba <sub>3</sub> (As $\bar{4}$ ) <sub>2</sub>	4.8256	LiYbS <sub>2</sub>
3.6820	Ni <sub>3</sub> (Ti <sub>0.83</sub> Ta <sub>0.17</sub> )	4.8311	Fe <sub>3</sub> Tb
3.6853	K <sub>2</sub> Pb(Cr $\bar{4}$ ) <sub>2</sub>	4.8545	Co <sub>3</sub> Y
3.6901	Ba <sub>3</sub> (V $\bar{4}$ ) <sub>2</sub>	4.8602	Co <sub>3</sub> Gd
3.6915	(Ni <sub>0.93</sub> Cu <sub>0.07</sub> ) <sub>3</sub> Ti	4.8630	Co <sub>3</sub> Er
3.7049	K <sub>2</sub> Sr(Cr $\bar{4}$ ) <sub>2</sub>	4.8631	Co <sub>3</sub> Tm
3.7265	Ba <sub>3</sub> (Cr $\bar{4}$ ) <sub>2</sub>	4.8655	Co <sub>3</sub> Tb
3.7287	Zn <sub>5</sub> (OH) <sub>8</sub> Cl <sub>2</sub> •H <sub>2</sub> $\bar{6}$	4.8661	Co <sub>3</sub> Dy
3.7306	U $\bar{6}$ F <sub>2</sub>	4.8678	Co <sub>3</sub> Ho
3.7377	K <sub>2</sub> Pb(Se $\bar{4}$ ) <sub>2</sub>	4.8688	NaPrSe <sub>2</sub>
3.7502	Ba <sub>3</sub> (P $\bar{4}$ ) <sub>2</sub>	4.8700	Ni <sub>3</sub> Pu
3.7562	PbRb <sub>2</sub> (Cr $\bar{4}$ ) <sub>2</sub>	4.8704	Co <sub>3</sub> Er
3.7565	BaRu $\bar{3}$	4.8704	Co <sub>3</sub> Sm
3.7591	BaK <sub>2</sub> (Cr $\bar{4}$ ) <sub>2</sub>	4.8865	Co <sub>3</sub> Nd
3.7601	3Mg(OH) <sub>2</sub> Fe(OH) <sub>3</sub> •3H <sub>2</sub> $\bar{6}$	4.8915	Co <sub>3</sub> Pr
3.7609	K <sub>2</sub> Pb(S $\bar{4}$ ) <sub>2</sub>	4.8973	FeCl <sub>2</sub>
3.7656	PbTl <sub>2</sub> (Cr $\bar{4}$ ) <sub>2</sub>	4.8988	NaNdSe <sub>2</sub>
3.7717	Ba <sub>3</sub> (Mn $\bar{4}$ ) <sub>2</sub>	4.8989	NaSmS <sub>2</sub>
3.7817	Np $\bar{2}$ F <sub>2</sub>	4.8995	MgCl <sub>2</sub>
3.7976	(NH <sub>4</sub> ) <sub>2</sub> Pb(Cr $\bar{4}$ ) <sub>2</sub>	4.9022	CdBr <sub>0.6</sub> (OH) <sub>1.4</sub>
3.7991	SrTl <sub>2</sub> (Cr $\bar{4}$ ) <sub>2</sub>	4.9048	KLaS <sub>2</sub>
3.8012	Rb <sub>2</sub> Sr(Cr $\bar{4}$ ) <sub>2</sub>	4.9080	CoCl <sub>2</sub>
3.8150	BaTl <sub>2</sub> (Cr $\bar{4}$ ) <sub>2</sub>	4.9239	NaTl $\bar{6}$
3.8226	(NH <sub>4</sub> ) <sub>2</sub> Pb(Se $\bar{4}$ ) <sub>2</sub>	4.9260	NiBr <sub>2</sub>
3.8239	Ba(NH <sub>4</sub> ) <sub>2</sub> (Cr $\bar{4}$ ) <sub>2</sub>	4.9282	NaEuS <sub>2</sub>
3.8258	BaRb <sub>2</sub> (Cr $\bar{4}$ ) <sub>2</sub>	4.9305	LiNi $\bar{6}$
3.8536	PbRb <sub>2</sub> (S $\bar{4}$ ) <sub>2</sub>	4.9340	Er $\bar{6}$ F
3.8592	(NH <sub>4</sub> ) <sub>2</sub> Sr(Cr $\bar{4}$ ) <sub>2</sub>	4.9351	FeBr <sub>2</sub>
3.9140	Pb(NH <sub>4</sub> ) <sub>2</sub> (S $\bar{4}$ ) <sub>2</sub>	4.9362	Yb $\bar{6}$ F
3.9571	PbTl <sub>2</sub> (S $\bar{4}$ ) <sub>2</sub>	4.9422	K <sub>2</sub> U $\bar{2}$ $\bar{6}$ <sub>7</sub>
3.9764	CaCN <sub>2</sub>	4.9500	NaSmSe <sub>2</sub>
4.0290	NaHF <sub>2</sub>	4.9563	NaGdS <sub>2</sub>
4.0463	CaCN <sub>2</sub>	4.9569	Y $\bar{6}$ F
4.0784	Ni <sub>3</sub> (Ti <sub>0.97</sub> Nb <sub>0.03</sub> )	4.9584	NaEuSe <sub>2</sub>
4.0894	C	4.9603	Ho $\bar{6}$ F
4.3909	LiHF <sub>2</sub>	4.9689	LiGa $\bar{6}$
4.4083	Cs <sub>2</sub> $\bar{6}$	4.9700	NaYb $\bar{6}$
4.4892	HCr $\bar{2}$	4.9737	Dy $\bar{6}$ F
4.4923	RbNp $\bar{2}$ F <sub>2</sub>	4.9745	Tb $\bar{6}$ F
4.4928	CdU $\bar{3}$ .63	4.9759	NaLu $\bar{6}$
4.4931	HCr $\bar{2}$	4.9773	Sm $\bar{6}$ F
4.4943	RbPu $\bar{2}$ F <sub>2</sub>	4.9811	Eu $\bar{6}$ F

R $\bar{3}m$  D $_{3d}^5$  No. 166 (continued)

## Inorganic (continued)

4.9812	NaTbS <sub>2</sub>	5.5892	TaSe <sub>2</sub>
4.9814	CoBr <sub>2</sub>	5.6440	CuFeO <sub>2</sub>
4.9814	GdOF	5.6517	CuGaO <sub>2</sub>
4.9828	NdOF	5.6747	N <sub>2</sub> W
4.9844	PrOF	5.6996	KScO <sub>2</sub>
4.9864	LaOF	5.7309	Cu(Ti <sub>0.5</sub> Ni <sub>0.5</sub> )O <sub>2</sub>
4.9876	LiCoO <sub>2</sub>	5.7492	CuCrO <sub>2</sub>
4.9939	CeCo <sub>3</sub>	5.8485	KCrS <sub>2</sub>
4.9957	NiCl <sub>2</sub>	5.9112	Al <sub>3</sub> Dy
4.9976	NaGdSe <sub>2</sub>	5.9138	RbScO <sub>2</sub>
5.0032	Na <sub>2</sub> PdO <sub>3</sub>	5.9310	CuAlO <sub>2</sub>
5.0075	NaDyS <sub>2</sub>	5.9369	Al <sub>3</sub> Ho
5.0126	NaYS <sub>2</sub>	5.9441	NaVO <sub>2</sub>
5.0217	NaTbSe <sub>2</sub>	6.0211	CuCoO <sub>2</sub>
5.0291	NaHoS <sub>2</sub>	6.1780	AgCrO <sub>2</sub>
5.0398	NiI <sub>2</sub>	6.8795	Bi <sub>2</sub> Se <sub>3</sub>
5.0449	ThNF	6.8836	Bi <sub>2</sub> Se <sub>3</sub>
5.0509	NaDySe <sub>2</sub>	6.9274	Bi <sub>2</sub> Te <sub>2</sub> Se
5.0525	NaInO <sub>2</sub>	6.9322	Bi <sub>2</sub> TeSe <sub>2</sub>
5.0558	NaYSe <sub>2</sub>	6.9394	Bi <sub>2</sub> Te <sub>3</sub>
5.0588	ZnI <sub>2</sub>	6.9463	Bi <sub>2</sub> Te <sub>3</sub>
5.0694	LiCrO <sub>2</sub>	6.9512	B <sub>5</sub> Mo <sub>2</sub>
5.0718	NaHoSe <sub>2</sub>	6.9513	Bi <sub>2</sub> Te <sub>3</sub>
5.0723	NaErS <sub>2</sub>	6.9516	Bi <sub>2</sub> Te <sub>2</sub> S
5.0766	LiAlO <sub>2</sub>	6.9533	Bi <sub>2</sub> Te <sub>3</sub>
5.0843	NaErSe <sub>2</sub>	6.9636	Bi <sub>2</sub> Te <sub>3</sub>
5.1390	NaScO <sub>2</sub>	6.9879	Bi <sub>2</sub> Se <sub>3</sub>
5.1622	Ca <sub>2</sub> N	7.0343	Bi <sub>1-x</sub> Ca <sub>x</sub> O <sub>1.5-0.5x</sub>
5.1622	KCeS <sub>2</sub>	7.0494	Sb <sub>2</sub> Te <sub>3</sub>
5.1761	LiVO <sub>2</sub>	7.0744	N <sub>4</sub> Th <sub>3</sub>
5.1925	Rb <sub>2</sub> U <sub>2</sub> O <sub>7</sub>	7.0963	Bi <sub>1-x</sub> Sr <sub>x</sub> O <sub>1.5-0.5x</sub>
5.1968	Na(Sn <sub>0.5</sub> Ni <sub>0.5</sub> )O <sub>2</sub>	7.1277	Ba <sub>x</sub> Bi <sub>1-x</sub> O <sub>1.5-0.5x</sub>
5.1971	KPrS <sub>2</sub>	7.1341	Sb <sub>2</sub> Te <sub>3</sub>
5.2033	K <sub>2</sub> CeO <sub>3</sub>	7.1506	Co <sub>7</sub> Er <sub>2</sub>
5.2301	NaInS <sub>2</sub>	7.2105	Gd
5.2470	KNdS <sub>2</sub>	7.2203	Sm
5.2593	NaInSe <sub>2</sub>	7.2240	Ce <sub>3</sub> Gd <sub>7</sub>
5.2779	NaFeO <sub>2</sub>	7.2293	Co <sub>7</sub> Gd <sub>2</sub>
5.2982	KSmS <sub>2</sub>	7.2391	Co <sub>7</sub> Y <sub>2</sub>
5.3247	KTbO <sub>2</sub>	7.2469	Co <sub>7</sub> Dy <sub>2</sub>
5.3277	NaNiO <sub>2</sub>	7.2476	Co <sub>7</sub> Tb <sub>2</sub>
5.3368	Co <sub>7</sub> Nb <sub>6</sub>	7.2494	Sm
5.3395	Al <sub>2</sub> Cu <sub>18</sub> (AsO <sub>4</sub> ) <sub>3</sub> (SO <sub>4</sub> ) <sub>3</sub> (OH) <sub>27</sub> •36H <sub>2</sub> O	7.2587	Co <sub>7</sub> Ho <sub>2</sub>
5.3396	KEuS <sub>2</sub>	7.2617	In <sub>2</sub> Se <sub>3</sub>
5.3415	CoNb	7.4745	Al <sub>4</sub> C <sub>3</sub>
5.3429	KTiO <sub>2</sub>	7.5080	4Mg(OH) <sub>2</sub> •Fe(OH) <sub>3</sub>
5.3484	NbS <sub>2</sub>	7.5484	4Zn(OH) <sub>2</sub> •Al(OH) <sub>3</sub>
5.3500	Na(Ti <sub>0.5</sub> Ni <sub>0.5</sub> )O <sub>2</sub>	7.5962	4Co(OH) <sub>2</sub> •Al(OH) <sub>3</sub>
5.3716	NaCrO <sub>2</sub>	7.6221	4Co(OH) <sub>2</sub> •Co(OH) <sub>3</sub>
5.3718	KGdS <sub>2</sub>	7.6221	4Mg(OH) <sub>2</sub> •Mn(OH) <sub>3</sub>
5.3790	Co <sub>7</sub> Mo <sub>6</sub>	7.6670	4Mg(OH) <sub>2</sub> •Al(OH) <sub>3</sub>
5.3949	Co <sub>7</sub> W <sub>6</sub>	7.7352	Ti <sub>1-x</sub> S
5.3986	KTbS <sub>2</sub>	7.7411	TiS
5.4045	Fe <sub>7</sub> Mo <sub>6</sub>	7.8531	CaSi <sub>2</sub>
5.4168	KDyS <sub>2</sub>	8.0157	[Na <sub>4</sub> (Ca, Mg) <sub>2</sub> Cl <sub>12</sub> ][Mg <sub>7</sub> Al <sub>4</sub> (OH) <sub>22</sub> ]
5.4264	NbSe <sub>2</sub>	8.0796	N <sub>0.85</sub> W
5.4274	Fe <sub>7</sub> W <sub>6</sub>	8.8177	(As <sub>1-x</sub> Sn <sub>x</sub> ) <sub>3</sub> Sn <sub>4</sub>
5.4331	KYS <sub>2</sub>	8.9926	(Fe, Cu) <sub>2</sub> •1.53[Mg <sub>0.7</sub> Al <sub>0.3</sub> (OH) <sub>2</sub> ]
5.4371	KHoS <sub>2</sub>	9.1589	Bi <sub>2</sub> GeTe <sub>4</sub>
5.4520	KErS <sub>2</sub>	9.1889	PbI <sub>2</sub>
5.4720	NaCrSe <sub>2</sub>	9.3608	Bi <sub>4</sub> TeS <sub>2</sub>
5.4888	Nb <sub>3</sub> I <sub>8</sub>	9.4111	Bi <sub>4+x</sub> (Te, Se, S) <sub>3-x</sub>
5.5011	Fe <sub>6</sub> Re <sub>6</sub> Si	9.4310	Bi <sub>4</sub> (S, Se) <sub>3</sub>
5.5045	KYbS <sub>2</sub>	9.4394	Bi <sub>4+x</sub> Se <sub>1-x</sub> S <sub>2</sub>
5.5049	Nb <sub>3</sub> Br <sub>8</sub>	9.4509	Bi <sub>4</sub> Se <sub>2</sub> S
5.5070	Co <sub>5.7</sub> Re <sub>6</sub> Si <sub>1.3</sub>	9.5442	Bi <sub>4+x</sub> (Te, Se, S) <sub>3-x</sub>
5.5110	TaS <sub>2</sub>	9.6437	GeSb <sub>2</sub> Te <sub>4</sub>
5.5350	RbTiO <sub>2</sub>	9.6752	SnSb <sub>2</sub> Te <sub>4</sub>
5.5449	Cu(Sn <sub>0.5</sub> Ni <sub>0.5</sub> )O <sub>2</sub>	9.7369	Al <sub>7</sub> Cu <sub>4</sub> Ni
5.5492	KInO <sub>2</sub>	9.8783	Sc <sub>2</sub> Te <sub>3</sub>
5.5718	TaSe <sub>2</sub>	9.9424	Fe <sub>3</sub> S <sub>4</sub>
5.5755	NaCrS <sub>2</sub>	10.0527	Ti <sub>5</sub> S <sub>8</sub>
5.5821	CuRhO <sub>2</sub>	10.7605	TaS <sub>2</sub>

R3m D<sub>3d</sub><sup>5</sup> No. 166 (continued)

## Inorganic (continued)

10.9320	TaSe <sub>2</sub>	26.6368	Bi <sub>7</sub> Te <sub>3</sub>
12.2449	Cu <sub>6</sub> S <sub>5</sub>	78.5714	Ba <sub>10</sub> (Mn,Zn) <sub>9</sub> Fe <sub>66</sub> <sup>δ</sup> <sub>108</sub>
12.3245	Al <sub>6</sub> C <sub>3</sub> N <sub>2</sub>	93.4184	Ba <sub>12</sub> (Mn,Zn) <sub>11</sub> Fe <sub>78</sub> <sup>δ</sup> <sub>140</sub>
13.4200	B <sub>12</sub> (Se <sub>4</sub> S) <sub>3</sub>	108.282	Ba <sub>14</sub> (Mn,Zn) <sub>13</sub> Fe <sub>90</sub> <sup>δ</sup> <sub>162</sub>
17.1535	Al <sub>8</sub> C <sub>3</sub> N <sub>4</sub>		

## Organic

0.9410	C <sub>5</sub> H <sub>5</sub> NH•SbF <sub>6</sub>	3.080	(NH <sub>3</sub> CH <sub>3</sub> ) <sub>2</sub> SnCl <sub>6</sub>
0.9715	C <sub>5</sub> H <sub>5</sub> NH•AsF <sub>6</sub>	3.194	(NH <sub>3</sub> CH <sub>3</sub> ) <sub>2</sub> PtCl <sub>6</sub>
0.9759	C <sub>5</sub> H <sub>5</sub> SI	3.630	CaCN <sub>2</sub>
0.9843	C <sub>5</sub> H <sub>5</sub> NH•PF <sub>6</sub>	3.9764	CaCN <sub>2</sub>
1.3245	Na <sub>2</sub> CaUO <sub>2</sub> (CO <sub>3</sub> ) <sub>3</sub> •6H <sub>2</sub> O	4.046	CaCN <sub>2</sub>
1.3439	CsCN	4.0894	C
1.4057	CH <sub>3</sub> •CH <sub>3</sub> •NH <sub>3</sub>	7.4745	Al <sub>4</sub> C <sub>3</sub>
1.9178	C <sub>8</sub> H <sub>6</sub>	12.3245	Al <sub>6</sub> C <sub>3</sub> N <sub>2</sub>
2.164	B <sub>4</sub> C	17.1535	Al <sub>8</sub> C <sub>3</sub> N <sub>4</sub>

$\bar{3}$ <sub>m</sub>

R3c D<sub>3d</sub><sup>6</sup> No. 167

Inorganic - 108  
Organic - 20

## Inorganic

0.5400	NaBO <sub>2</sub>	2.7105	GaFeO <sub>3</sub>
0.5435	KBS <sub>2</sub>	2.7298	Al <sub>2</sub> O <sub>3</sub>
0.5749	KBO <sub>2</sub>	2.7301	Fe <sub>2</sub> O <sub>3</sub>
0.6092	H <sub>3</sub> B <sub>3</sub> N <sub>3</sub> F <sub>3</sub>	2.7305	Al <sub>2</sub> O <sub>3</sub>
1.0059	CrCl <sub>3</sub> •6H <sub>2</sub> O	2.7333	Fe <sub>2</sub> O <sub>3</sub>
1.0060	AlCl <sub>3</sub> •6H <sub>2</sub> O	2.7402	Cr <sub>2</sub> O <sub>3</sub>
1.1644	FeK <sub>3</sub> NaCl <sub>6</sub>	2.7413	Cr <sub>2</sub> O <sub>3</sub>
1.1691	FeK <sub>3</sub> NaCl <sub>6</sub>	2.7430	(Cr,V,Fe) <sub>2</sub> O <sub>3</sub>
1.1928	Rb <sub>4</sub> CdBr <sub>6</sub>	2.7470	Cr <sub>2</sub> O <sub>3</sub>
1.2143	K <sub>4</sub> CdBr <sub>6</sub>	2.7667	MoF <sub>3</sub>
1.2146	K <sub>4</sub> CdCl <sub>6</sub>	2.7698	RuF <sub>3</sub>
1.2218	Sr <sub>4</sub> PtO <sub>6</sub>	2.7860	RhF <sub>3</sub>
1.2248	K <sub>4</sub> CdCl <sub>6</sub>	2.8016	V <sub>2</sub> O <sub>3</sub>
1.2397	K <sub>4</sub> MnCl <sub>6</sub>	2.8050	IrF <sub>3</sub>
1.2436	(NH <sub>4</sub> ) <sub>4</sub> CdBr <sub>6</sub>	2.8185	PdF <sub>3</sub>
1.2480	Rb <sub>4</sub> CdCl <sub>6</sub>	2.8239	V <sub>2</sub> O <sub>3</sub>
1.2518	(NH <sub>4</sub> ) <sub>4</sub> CdCl <sub>6</sub>	2.8377	CNi <sub>3</sub>
1.2570	K <sub>4</sub> CdCl <sub>6</sub>	2.9184	Mn <sub>2</sub> O <sub>3</sub>
1.2579	(NH <sub>4</sub> ) <sub>4</sub> CdCl <sub>6</sub>	3.0800	Mg <sub>2</sub> B <sub>12</sub> O <sub>20</sub> •15H <sub>2</sub> O
1.2645	Rb <sub>4</sub> CdCl <sub>6</sub>	3.1117	CrBO <sub>3</sub>
1.2732	K <sub>4</sub> PbF <sub>6</sub>	3.1259	Fe <sub>0.9</sub> Ga <sub>0.1</sub> BO <sub>3</sub>
1.2815	FeF <sub>3</sub>	3.1314	VB <sub>3</sub>
1.3110	CoF <sub>3</sub>	3.1906	TiBO <sub>3</sub>
1.3959	RhF <sub>3</sub>	3.1980	NiCO <sub>3</sub>
1.4011	PdF <sub>3</sub>	3.2024	NiCO <sub>3</sub>
1.4251	Cs <sub>3</sub> Tl <sub>2</sub> Cl <sub>9</sub>	3.2046	InBO <sub>3</sub>
1.4297	Cs <sub>3</sub> Tl <sub>2</sub> Cl <sub>9</sub>	3.2112	CoCO <sub>3</sub>
1.8716	SrCO <sub>3</sub>	3.2142	CoCO <sub>3</sub>
2.0171	RbUO <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub>	3.2176	ScBO <sub>3</sub>
2.0239	CsUO <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub>	3.2194	ScBO <sub>3</sub>
2.1019	NiBa <sub>3</sub> O <sub>4</sub>	3.2202	ZnCO <sub>3</sub>
2.5001	TiF <sub>3</sub>	3.2277	CuCO <sub>3</sub>
2.5646	FeF <sub>3</sub>	3.2292	ZnCO <sub>3</sub>
2.5809	Tl <sub>2</sub> O <sub>3</sub>	3.2370	CoCO <sub>3</sub>
2.5919	VF <sub>3</sub>	3.2394	MgCO <sub>3</sub>
2.5934	GaF <sub>3</sub>	3.2411	MgCO <sub>3</sub>
2.6100	TlInO <sub>3</sub>	3.2428	InBO <sub>3</sub>
2.6252	CoF <sub>3</sub>	3.2516	LiNO <sub>3</sub>
2.6444	In <sub>2</sub> O <sub>3</sub>	3.2750	FeCO <sub>3</sub>
2.6446	Tl <sub>2</sub> O <sub>3</sub>	3.2750	MnCO <sub>3</sub>
2.6494	Ti <sub>2</sub> O <sub>3</sub>	3.2764	(Mn,Fe,Zn)CO <sub>3</sub>
2.6498	CrF <sub>3</sub>	3.2773	FeCO <sub>3</sub>
2.6510	Tl <sub>2</sub> O <sub>3</sub>	3.2790	MnCO <sub>3</sub>
2.6628	InF <sub>3</sub>	3.3002	LuBO <sub>3</sub>
2.6669	InScO <sub>3</sub>	3.3043	FeCO <sub>3</sub>
2.6747	InFeO <sub>3</sub>	3.3055	CdCO <sub>3</sub>
2.6988	Ga <sub>2</sub> O <sub>3</sub>	3.3123	CdCO <sub>3</sub>
2.6988	Rh <sub>2</sub> O <sub>3</sub>	3.3193	NaN <sub>3</sub>
2.6994	Yb <sub>2</sub> S <sub>3</sub>	3.4012	YBO <sub>3</sub>
2.7058	Lu <sub>2</sub> S <sub>3</sub>	3.4169	CaCO <sub>3</sub>



R3c  $D_{3d}^6$  No. 167 (continued)

## Inorganic (continued)

3.4190	CaC $\theta_3$	10.3833	Ca $_4$ Fe $_2$ Fe $_{18}\theta_{33}$
3.5756	Ca $_3$ (P $\theta_4$ ) $_2$	15.6716	CaFe $_4\theta_7$
3.9080	MnPb $_3$ (Si $_2\theta_7$ ) $_3$	15.8333	Ca $_4$ Fe $_{14}\theta_{25}$
5.4170	BaB $_2\theta_4$	25.0000	Mn $_9$ Mg $_4$ Zn $_2$ As $_2$ Si $_2\theta_{17}$ ( $\theta$ H) $_{14}$

## Organic

0.7547	C $_3$ H $_3$ N $_3$	3.237	CoC $\theta_3$
0.7739	SC(NH $_2$ ) $_2 \cdot x$	3.2394	MgC $\theta_3$
0.8980	[Cr(NH $_2$ C $\theta$ NH $_2$ ) $_6$ ]Cl $_3$	3.2750	FeC $\theta_3$
0.9134	[Fe(NH $_2$ C $\theta$ NH $_2$ ) $_6$ ]Cl $_3$	3.2750	MnC $\theta_3$
1.872	SrC $\theta_3$	3.2764	(Mn,Fe,Zn)C $\theta_3$
2.8377	Ni $_3$ C	3.2773	FeC $\theta_3$
3.1980	NiC $\theta_3$	3.3043	FeC $\theta_3$
3.2142	CoC $\theta_3$	3.306	CdC $\theta_3$
3.2202	ZnC $\theta_3$	3.4169	CaC $\theta_3$
3.227	CuC $\theta_3$	3.4190	CaC $\theta_3$

6 P6  $C_6^1$  No. 168 Inorganic - 2  
Organic - 1

## Inorganic

1.6455	LiRh	3.7686	NbSe $_2$
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## Organic

0.4187	U $\theta_2$ (C $_6$ H $_4\theta$ H $\theta\theta$ ) $_2 \cdot 3$ H $_2\theta$
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6 P6 $_1$   $C_6^2$  No. 169 (includes P6 $_5$  No. 170) Inorganic - 3  
Organic - 6

## Inorganic

2.7145	In $_2$ Se $_3$	13.6626	Ca $_2$ Si $_4\theta_{10} \cdot 4$ H $_2\theta$
2.8340	Ga $_2$ S $_3$		

## Organic

1.517	(C $_6$ H $_2$ )Br $\cdot$ (N $\theta_2$ ) $_3$	2.6305	[(CH $_3$ ) $_2$ C] $_3$ C $_3$
1.779	C $_6$ H $_3$ (C $\theta\theta$ C $_2$ H $_5$ ) $_3$	2.729	[Co(C $_6$ H $_{14}$ N $_2$ ) $_3$ ]Cl $_3 \cdot 4$ H $_2\theta$
2.290	C $_{18}$ H $_{24}$	3.226	N(C $_2$ H $_4 \cdot$ NH $_3$ Cl) $_3 \cdot$ HCl+H $_2\theta$

6 P6 $_5$   $C_6^3$  No. 170 (see No. 169)

.....

6 P6 $_2$   $C_6^4$  No. 171 (includes P6 $_4$  No. 172) Inorganic - 0  
Organic - 1

## Inorganic

.....

## Organic

2.0352	2C $_{33}$ H $_{36}\theta_6 \cdot$ C $_6$ H $_{14}$
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6 P6 $_4$   $C_6^5$  No. 172 (see No. 171)

.....

6 P6 $_3$   $C_6^6$  No. 173 Inorganic - 24  
Organic - 7

## Inorganic

0.4031	Na $_6$ CaC $\theta_3$ (Al $_6$ Si $_6\theta_{24}$ ) $\cdot 2$ H $_2\theta$	0.4068	CaNa $_3$ (AlSi $\theta_4$ ) $_3$ C $\theta_3$
0.4053	Na $_5$ (Al $_3$ Si $_3\theta_{12}$ )C $\theta_3$	0.4068	Na $_5$ (Al $_3$ Si $_3\theta_{12}$ )C $\theta_3$

P6<sub>3</sub> C<sub>6</sub><sup>6</sup> No. 173 (continued)

## Inorganic (continued)

0.4072	CaNa <sub>3</sub> (AlSi <sub>6</sub> ) <sub>3</sub> C <sub>6</sub>	0.9433	LiI <sub>3</sub>
0.5566	Ca <sub>4</sub> Mn <sub>3-x</sub> [(B <sub>6</sub> ) <sub>2</sub> (C <sub>6</sub> )(OH) <sub>3</sub> ]	0.9438	LiI <sub>3</sub>
0.5584	(Na,K)AlSi <sub>6</sub>	0.9494	Ca <sub>3</sub> Mn(S <sub>6</sub> )(C <sub>6</sub> )(OH) <sub>6</sub> •12H <sub>2</sub> O
0.6118	Tl <sub>3</sub> P <sub>6</sub>	1.0447	NaHP <sub>6</sub> NH <sub>2</sub>
0.6146	Tl <sub>3</sub> As <sub>6</sub>	1.0715	BBr <sub>3</sub>
0.6809	Pb <sub>5</sub> Cl(As <sub>6</sub> ) <sub>3</sub>	1.0773	BCl <sub>3</sub>
0.8357	NaAlSi <sub>6</sub>	1.2025	In <sub>2</sub> Se <sub>3</sub>
0.8397	KNa <sub>3</sub> [(Al <sub>2</sub> Si) <sub>4</sub> ] <sub>4</sub>	1.6764	KLiS <sub>6</sub>
0.8426	NaAlSi <sub>6</sub>	1.6844	KAlSi <sub>6</sub>
0.9406	Ca <sub>3</sub> H <sub>2</sub> (C <sub>6</sub> )(S <sub>6</sub> )Si <sub>6</sub> •13H <sub>2</sub> O	1.8068	Al <sub>5</sub> W

## Organic

0.5804	NaI <sub>3</sub> [(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> ]	0.7788	[Co(NH <sub>2</sub> CHCH <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>3</sub> ]Br <sub>3</sub>
0.665	C <sub>6</sub> H <sub>10</sub> N <sub>6</sub> H	1.104	CHI <sub>3</sub>
0.6791	(CH <sub>3</sub> ) <sub>4</sub> NNIBr <sub>3</sub>	4.1607	C <sub>37</sub> H <sub>51</sub> I <sub>6</sub>
0.7752	Co(C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> ) <sub>3</sub> Br <sub>3</sub>		

6

P6 C<sub>3h</sub><sup>1</sup> No. 174Inorganic - 7  
Organic - 0

## Inorganic

0.5849	NaLuF <sub>4</sub>	0.6113	NaPrF <sub>4</sub>
0.5889	NaHoF <sub>4</sub>	0.9997	Zr <sub>3</sub> S <sub>2</sub>
0.5959	NaTbF <sub>4</sub>	1.2228	Li <sub>2</sub> O <sub>2</sub>
0.6084	NaNdF <sub>4</sub>		

## Organic

.....

6

P6/m C<sub>6h</sub><sup>1</sup> No. 175Inorganic - 0  
Organic - 0

.....

6

P6<sub>3</sub>/m C<sub>6h</sub><sup>2</sup> No. 176Inorganic - 101  
Organic - 20

## Inorganic

0.3377	Mg <sub>3</sub> (OH,F) <sub>3</sub> B <sub>6</sub>	0.5805	UCl <sub>3</sub>
0.3418	Nb <sub>3</sub> Ie <sub>4</sub>	0.5806	AcBr <sub>3</sub>
0.3467	Nb <sub>3</sub> Se <sub>4</sub>	0.5811	Pr(OH) <sub>3</sub>
0.3607	Th <sub>7</sub> S <sub>12</sub>	0.5825	Nd(OH) <sub>3</sub>
0.3656	Th <sub>7</sub> Se <sub>12</sub>	0.5846	LaCl <sub>3</sub>
0.3826	N <sub>4</sub> Si <sub>3</sub>	0.5869	NaTmF <sub>4</sub>
0.3931	PbSb <sub>2</sub> S <sub>4</sub>	0.5903	La(OH) <sub>3</sub>
0.5511	Pu(Br <sub>0.8</sub> Cl <sub>0.2</sub> ) <sub>3</sub>	0.5910	La(OH) <sub>3</sub>
0.5530	PrBr <sub>3</sub>	0.5971	AcCl <sub>3</sub>
0.5532	CfCl <sub>3</sub>	0.6016	NaSmF <sub>4</sub>
0.5535	NpBr <sub>3</sub>	0.6595	3CsCl•H <sub>3</sub> OHCl <sub>2</sub>
0.5575	GdCl <sub>3</sub>	0.6957	Ca <sub>5</sub> (P <sub>6</sub> ) <sub>3</sub> Br
0.5588	CeBr <sub>3</sub>	0.7050	Ca <sub>8.4</sub> Mn <sub>1.1</sub> Fe <sub>0.5</sub> P <sub>6</sub> O <sub>24</sub> (OH) <sub>2</sub>
0.5592	UBr <sub>3</sub>	0.7097	Ca <sub>5</sub> F(As <sub>6</sub> ) <sub>3</sub>
0.5609	EuCl <sub>3</sub>	0.7100	Pb <sub>5</sub> Cl(V <sub>6</sub> ) <sub>3</sub>
0.5627	Yb(OH) <sub>3</sub>	0.7108	Pb <sub>5</sub> Cl(V <sub>6</sub> ) <sub>3</sub>
0.5653	SmCl <sub>3</sub>	0.7109	(Y,Ca) <sub>5</sub> [(Si,Al,P) <sub>6</sub> ] <sub>3</sub> (OH,F)
0.5657	Y(OH) <sub>3</sub>	0.7119	Pb <sub>5</sub> Cl(V <sub>6</sub> ) <sub>3</sub>
0.5661	LaBr <sub>3</sub>	0.7122	Ca <sub>9</sub> BaCl <sub>2</sub> (P <sub>6</sub> ) <sub>6</sub>
0.5688	Sm(OH) <sub>3</sub>	0.7122	Ca <sub>9</sub> PbCl <sub>2</sub> (P <sub>6</sub> ) <sub>6</sub>
0.5727	Eu(OH) <sub>3</sub>	0.7161	Ca <sub>9</sub> MgCl <sub>2</sub> (P <sub>6</sub> ) <sub>6</sub>
0.5729	AmCl <sub>3</sub>	0.7169	Ca <sub>9</sub> NiCl <sub>2</sub> (P <sub>6</sub> ) <sub>6</sub>
0.5732	NdCl <sub>3</sub>	0.7195	Ca <sub>5</sub> Cl(P <sub>6</sub> ) <sub>3</sub>
0.5735	PrCl <sub>3</sub>	0.7225	Sr <sub>5</sub> Cl(Cr <sub>6</sub> ) <sub>3</sub>
0.5738	CmCl <sub>3</sub>	0.7239	Ca <sub>4</sub> Na <sub>6</sub> (S <sub>6</sub> ) <sub>6</sub> F <sub>2</sub>
0.5743	PuCl <sub>3</sub>	0.7239	Ca <sub>5</sub> OH(Cr <sub>6</sub> ) <sub>3</sub>
0.5753	AmCl <sub>3</sub>	0.7245	Ca <sub>10.5</sub> (P <sub>6</sub> ) <sub>3</sub> (Si <sub>6</sub> ) <sub>2</sub> (S <sub>6</sub> ) <sub>2</sub> F <sub>2</sub>
0.5770	NpCl <sub>3</sub>	0.7248	Ca <sub>8</sub> Na <sub>2</sub> (P <sub>6</sub> ) <sub>4</sub> (S <sub>6</sub> ) <sub>2</sub> F <sub>2</sub>
0.5788	CeCl <sub>3</sub>	0.7256	Pb <sub>5</sub> Cl(As <sub>6</sub> ) <sub>3</sub>

P<sub>6</sub><sub>3</sub>/m C<sub>6h</sub><sup>2</sup> No. 176 (continued)

Inorganic

0.7262	Ca <sub>10.5</sub> (P <sub>6</sub> ) <sub>5</sub> (S <sub>6</sub> )F <sub>2</sub>	0.7364	Pb <sub>5</sub> OH(P <sub>6</sub> ) <sub>3</sub>
0.7271	Ca <sub>10</sub> θ(P <sub>6</sub> ) <sub>6</sub>	0.7372	Ca <sub>5</sub> OH(P <sub>6</sub> ) <sub>3</sub>
0.7288	(Ca,Mn) <sub>6</sub> Ca <sub>4</sub> F <sub>2</sub> (P <sub>6</sub> ) <sub>6</sub>	0.7373	Ca <sub>10</sub> (P <sub>6</sub> ) <sub>4</sub> (S <sub>6</sub> ) <sub>4</sub> (OH) <sub>2</sub>
0.7290	Ca <sub>9</sub> Pbθ(P <sub>6</sub> ) <sub>6</sub>	0.7387	Ba <sub>5</sub> Cl(Cr <sub>6</sub> ) <sub>3</sub>
0.7291	Ca <sub>9</sub> Srθ(P <sub>6</sub> ) <sub>6</sub>	0.7388	Ca <sub>10</sub> θ(P <sub>6</sub> ) <sub>6</sub>
0.7292	(Ca,Sr) <sub>6</sub> Ca <sub>4</sub> (F,OH,θ) <sub>2</sub> (P,As) <sub>6</sub> θ <sub>24</sub>	0.7392	Sr <sub>5</sub> (OH)(P <sub>6</sub> ) <sub>3</sub>
0.7295	Ce <sub>2</sub> (S <sub>6</sub> ) <sub>3</sub> •9H <sub>2</sub> θ	0.7404	La <sub>2</sub> (S <sub>6</sub> ) <sub>3</sub> •9H <sub>2</sub> θ
0.7302	Ca <sub>9</sub> Niθ(P <sub>6</sub> ) <sub>6</sub>	0.7438	3Ca <sub>3</sub> (P <sub>6</sub> ) <sub>2</sub> •2H <sub>2</sub> θ
0.7304	Ca <sub>9.5</sub> (P <sub>6</sub> ) <sub>3</sub> (S <sub>6</sub> ) <sub>4</sub> (S <sub>6</sub> ) <sub>2</sub> F <sub>2</sub>	0.7455	Sr <sub>5</sub> (OH)(P <sub>6</sub> ) <sub>3</sub>
0.7305	(Ca,Mn) <sub>5</sub> P <sub>3</sub> θ <sub>12</sub> F	0.7497	Ca <sub>10</sub> θθ <sub>3</sub> (P <sub>6</sub> ) <sub>6</sub>
0.7305	(Ce,Ca,Na) <sub>5</sub> (F,OH)[(Si,P)θ <sub>4</sub> ] <sub>3</sub>	0.7556	Ba <sub>5</sub> OH(P <sub>6</sub> ) <sub>3</sub>
0.7306	Ca <sub>5</sub> OH(P <sub>6</sub> ) <sub>3</sub>	0.9551	AlBθ <sub>3</sub>
0.7322	(Ca,Ln) <sub>2.06</sub> (Si,Al,P) <sub>1.14</sub> (θ,OH,F) <sub>5.37</sub>	1.0647	BI <sub>3</sub>
0.7327	Ca <sub>10</sub> F <sub>2</sub> (S <sub>6</sub> ) <sub>3</sub> (S <sub>6</sub> ) <sub>3</sub>	1.4757	K <sub>2</sub> ZrSi <sub>3</sub> θ <sub>9</sub>
0.7336	Cd <sub>5</sub> OH(P <sub>6</sub> ) <sub>3</sub>	2.0200	KNa <sub>22</sub> Cl(Cθ <sub>3</sub> ) <sub>2</sub> (S <sub>6</sub> ) <sub>9</sub>
0.7338	Ca <sub>9</sub> Na <sub>2</sub> (P <sub>6</sub> ) <sub>4</sub> (S <sub>6</sub> ) <sub>4</sub> (S <sub>6</sub> )F <sub>2</sub>	2.0249	KNa <sub>22</sub> Cl(Cθ <sub>3</sub> ) <sub>2</sub> (S <sub>6</sub> ) <sub>9</sub>
0.7343	Ca <sub>5</sub> F(P <sub>6</sub> ) <sub>3</sub>	2.2584	(NH <sub>4</sub> ) <sub>3</sub> W <sub>2</sub> Cl <sub>9</sub>
0.7347	Ca <sub>5</sub> F(P <sub>6</sub> ) <sub>3</sub>	2.2672	K <sub>3</sub> W <sub>2</sub> Cl <sub>9</sub>
0.7347	Pb <sub>5</sub> Cl(P <sub>6</sub> ) <sub>3</sub>	2.2839	Tl <sub>3</sub> W <sub>2</sub> Cl <sub>9</sub>
0.7349	[RE,Ca,Mn] <sub>5</sub> [(S <sub>6</sub> ),(P <sub>6</sub> )] <sub>3</sub> (F,OH)	2.3211	Cs <sub>3</sub> W <sub>2</sub> Cl <sub>9</sub>
0.7357	Pb <sub>5</sub> (F,Cl)(P <sub>6</sub> ) <sub>3</sub>	2.3412	Rb <sub>3</sub> W <sub>2</sub> Cl <sub>9</sub>
0.7360	Ca <sub>5</sub> Pb <sub>5</sub> (P <sub>6</sub> ) <sub>6</sub> (OH) <sub>2</sub>		

Organic

0.505	Nd(C <sub>2</sub> H <sub>5</sub> S <sub>6</sub> ) <sub>3</sub> •9H <sub>2</sub> θ	0.750	Ca <sub>10</sub> θθ <sub>3</sub> (P <sub>6</sub> ) <sub>6</sub>
0.505	La(C <sub>2</sub> H <sub>5</sub> S <sub>6</sub> ) <sub>3</sub> •9H <sub>2</sub> θ	0.7986	NaI•3CH <sub>3</sub> OH
0.506	Dy(C <sub>2</sub> H <sub>5</sub> S <sub>6</sub> ) <sub>3</sub> •9H <sub>2</sub> θ	0.8306	(NH <sub>2</sub> •NH) <sub>3</sub> C•Cl
0.506	Pr(C <sub>2</sub> H <sub>5</sub> S <sub>6</sub> ) <sub>3</sub> •9H <sub>2</sub> θ	0.845	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>
0.506	Ce(C <sub>2</sub> H <sub>5</sub> S <sub>6</sub> ) <sub>3</sub> •9H <sub>2</sub> θ	1.1555	(C <sub>5</sub> H <sub>5</sub> ) <sub>3</sub> Ni <sub>3</sub> (Cθ) <sub>2</sub>
0.5063	Ho[(C <sub>2</sub> H <sub>5</sub> S <sub>6</sub> ) <sub>3</sub> •9H <sub>2</sub> θ]	1.5107	Mo(C <sub>2</sub> H <sub>2</sub> S <sub>2</sub> ) <sub>3</sub>
0.5068	Y(C <sub>2</sub> H <sub>5</sub> S <sub>6</sub> ) <sub>3</sub> •9H <sub>2</sub> θ	1.5452	(CH <sub>2</sub> •CH <sub>2</sub> ) <sub>3</sub> N <sub>2</sub>
0.507	Gd(C <sub>2</sub> H <sub>5</sub> S <sub>6</sub> ) <sub>3</sub> •9H <sub>2</sub> θ	2.020	9Na <sub>2</sub> S <sub>6</sub> •2Na <sub>2</sub> Cθ <sub>3</sub> •KCl
0.507	Sm(C <sub>2</sub> H <sub>5</sub> S <sub>6</sub> ) <sub>3</sub> •9H <sub>2</sub> θ	2.024	KNa <sub>22</sub> Cl(Cθ <sub>3</sub> ) <sub>2</sub> (S <sub>6</sub> ) <sub>9</sub>
0.662	(CH <sub>3</sub> ) <sub>2</sub> CNθH	2.4775	Fe <sub>2</sub> (Cθ) <sub>9</sub>

6 2 2

P6<sub>22</sub> D<sub>6</sub><sup>1</sup> No. 177

Inorganic - 2  
Organic - 0

Inorganic

0.9169	(Ca,Th)P <sub>6</sub> •H <sub>2</sub> θ	2.3932	NH <sub>4</sub> Cl•As <sub>2</sub> θ <sub>3</sub> •0.5H <sub>2</sub> θ
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Organic

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6 2 2

P6<sub>122</sub> D<sub>6</sub><sup>2</sup> No. 178 (includes P6<sub>522</sub> No. 179)

Inorganic - 3  
Organic - 9

Inorganic

2.5000	CsCuCl <sub>3</sub>	2.5191	CsCuCl <sub>3</sub>
2.5050	Ba(Nθ <sub>2</sub> ) <sub>2</sub> •H <sub>2</sub> θ		

Organic

1.3197	5CH <sub>4</sub> N <sub>2</sub> θ•C <sub>8</sub> H <sub>14</sub> θ <sub>4</sub>	1.9747	C <sub>32</sub> H <sub>47</sub> N <sub>6</sub> θ <sub>6</sub> Cl <sub>0.2</sub> I <sub>0.8</sub> •C <sub>2</sub> H <sub>5</sub> OH•1.5H <sub>2</sub> θ
1.3372	(C <sub>16</sub> H <sub>34</sub> )•(NH <sub>2</sub> CθNH <sub>2</sub> )	1.9927	C <sub>32</sub> H <sub>47</sub> N <sub>6</sub> θ <sub>6</sub> Cl•C <sub>2</sub> H <sub>5</sub> OH•1.5H <sub>2</sub> θ
1.9399	C <sub>32</sub> H <sub>48</sub> N <sub>6</sub> θ <sub>6</sub> •x•C <sub>2</sub> H <sub>5</sub> θH•yH <sub>2</sub> θ	2.020	C <sub>32</sub> H <sub>48</sub> N <sub>6</sub> θ <sub>6</sub> •C <sub>2</sub> H <sub>5</sub> θH•1.5H <sub>2</sub> θ
1.9502	C <sub>32</sub> H <sub>47</sub> N <sub>6</sub> θ <sub>6</sub> Cl•x•C <sub>2</sub> H <sub>5</sub> θH•yH <sub>2</sub> θ	10.379	(-S-CH <sub>2</sub> -CH(NH <sub>2</sub> )CθθH) <sub>2</sub>
1.9574	C <sub>32</sub> H <sub>47</sub> N <sub>6</sub> θ <sub>6</sub> Cl <sub>0.2</sub> I <sub>0.8</sub> •C <sub>2</sub> H <sub>5</sub> θH•xH <sub>2</sub> θ		

6 2 2

P6<sub>522</sub> D<sub>6</sub><sup>3</sup> No. 179 (see No. 178)

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6 2 2	P <sub>6</sub> <sub>2</sub> 22	D <sub>6</sub> <sup>4</sup>	No. 180 (includes P <sub>6</sub> <sub>4</sub> 22 No. 181)	Inorganic - 24 Organic - 2
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## Inorganic

0.6572	K <sub>5</sub> CoW <sub>12</sub> O <sub>40</sub> •20H <sub>2</sub> O	1.3742	NbSi <sub>2</sub>
0.9070	CaS <sub>6</sub>	1.3837	(Ga <sub>0.3</sub> Ge <sub>0.7</sub> ) <sub>2</sub> Mo
0.9083	NdP <sub>6</sub>	1.3896	HfSn <sub>2</sub>
0.9127	CeP <sub>6</sub>	1.4184	(Al <sub>1</sub> Si) <sub>2</sub> Cr
0.9134	LaP <sub>6</sub>	1.4353	Al <sub>0.75</sub> MnSi <sub>1.25</sub>
0.9187	GdP <sub>6</sub> •H <sub>2</sub> O	1.4362	CrSi <sub>2</sub>
0.9211	AcP <sub>6</sub> •0.5H <sub>2</sub> O	1.5080	Hg <sub>2</sub> Ge <sub>2</sub> NaI
1.0916	Si <sub>6</sub>	1.6964	Be <sub>2</sub> Fe <sub>2</sub> (Mn,Mg,Na)(P <sub>6</sub> ) <sub>4</sub> •6H <sub>2</sub> O
1.1050	AlP <sub>6</sub>	2.1347	LiAlSi <sub>6</sub>
1.3655	Ge <sub>2</sub> Nb	2.5472	Mg <sub>2</sub> Ni
1.3724	NbSi <sub>2</sub>	2.5808	Mo <sub>2</sub> Sn <sub>3</sub>
1.3738	Si <sub>2</sub> Ta	3.1157	Cu <sub>3</sub> Si

## Organic

5.0291	C <sub>30</sub> H <sub>41</sub> N <sub>3</sub> O <sub>7</sub>	6.086	C(CH <sub>2</sub> O) <sub>4</sub> (CHC <sub>6</sub> H <sub>5</sub> ) <sub>2</sub>
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6 2 2	P <sub>6</sub> <sub>4</sub> 22	D <sub>6</sub> <sup>5</sup>	No. 181 (see No. 180)	
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6 2 2	P <sub>6</sub> <sub>3</sub> 22	D <sub>6</sub> <sup>6</sup>	No. 182	Inorganic - 17 Organic - 1
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## Inorganic

0.3174	KAlSi <sub>6</sub>	1.6819	BaAl <sub>2</sub> Si <sub>4</sub>
0.4534	RuBr <sub>3</sub>	1.6839	BaAl <sub>2</sub> Si <sub>4</sub>
0.4549	TiI <sub>3</sub>	1.6911	BaGa <sub>2</sub> Si <sub>4</sub>
0.4594	MoBr <sub>3</sub>	1.8234	Cs <sub>2</sub> S <sub>2</sub> Si <sub>6</sub>
0.4900	Pu <sub>2</sub> Zn <sub>9</sub>	1.8326	As <sub>2</sub> Ni <sub>5</sub>
0.9345	Fe <sub>3</sub> N	1.8716	As <sub>2</sub> Pd <sub>5</sub>
1.1931	YbBe <sub>3</sub>	2.1297	UTe <sub>3</sub> Si <sub>10</sub>
1.6613	MgZn <sub>5</sub>	3.2133	Be <sub>4</sub> Mg <sub>4</sub> (Al,Fe) <sub>16</sub> Si <sub>32</sub>
1.6801	BaAl <sub>2</sub> Si <sub>4</sub>		

## Organic

1.2864	[Ni(NH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -NH <sub>2</sub> ) <sub>3</sub> ](NO <sub>3</sub> ) <sub>2</sub>
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6 m m	P6mm	C <sub>6v</sub> <sup>1</sup>	No. 183	Inorganic - 3 Organic - 1
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## Inorganic

0.8218	Co <sub>6</sub> Er	1.4971	AuCN
1.4599	Ca <sub>2</sub> [Co(NO <sub>2</sub> ) <sub>6</sub> ]Br•8H <sub>2</sub> O		

## Organic

1.4971	AuCN
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6 m m	P6cc	C <sub>6v</sub> <sup>2</sup>	No. 184	Inorganic - 0 Organic - 0
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6 m m	P6 <sub>3</sub> cm	C <sub>6v</sub> <sup>3</sup>	No. 185	Inorganic - 6 Organic - 1
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## Inorganic

1.0279	LaF <sub>3</sub>	1.9175	ScMn <sub>6</sub>
1.8695	ErMn <sub>6</sub>	2.6434	(Mg <sub>1.6</sub> Al <sub>1.0</sub> Fe <sub>0.4</sub> )(SiAl <sub>5</sub> )(OH) <sub>4</sub>
1.8847	LuMn <sub>6</sub>	2.7302	(Mg,Fe) <sub>3</sub> (OH) <sub>4</sub> Si <sub>2</sub> Si <sub>5</sub>

$P6_3cm$   $C_{6v}^3$  No. 185 (continued)

## Organic

0.6860  $(C_6H_{11})_3C_3H_3O_3$

6 mm

$P6_3mc$   $C_{6v}^4$  No. 186

Inorganic - 106  
Organic - 14

## Inorganic

0.4338	$Ca_5Pb_3$	1.6291	$MgTe$
0.5459	$Na_2OsF_6$	1.6297	$CdS$
0.5526	$Na_2RuF_6$	1.6302	$CdSe$
0.5601	$Na_2RhF_6$	1.6311	$MnSe$
0.5635	$Na_2CrF_6$	1.6318	$ZnAl_2S_4$
0.5688	$Na_2PdF_6$	1.6332	$(Zn, Mn, Fe)S$
0.5763	$Nd(BrO_3)_3 \cdot 9H_2O$	1.6354	$AgI$
0.6244	$Fe_3Th_7$	1.6355	$AgI$
0.6249	$Ir_3Th_7$	1.6358	$Ga_2S_3$
0.6275	$RhTh_2$	1.6358	$ZnS$
0.6277	$Co_3Th_7$	1.6368	$CdTe$
0.6277	$Os_3Th_7$	1.6384	$AsIn$
0.6312	$B_3Ru_7$	1.6404	$CuBr$
0.6318	$Ni_3Th_7$	1.6409	$SiC$
0.6381	$Ce_7Ni_3$	1.6421	$K_2CrF_6$
0.6441	$B_3Tc_7$	1.6450	$CuI$
0.6596	$C_3Fe_7$	1.6452	$K_2TiF_6$
0.6928	$LiMnO_4 \cdot 3H_2O$	1.6471	$BN$
0.7030	$LiClO_4 \cdot 3H_2O$	1.6490	$K_2MnF_6$
0.7315	$LiIO_3 \cdot H_2O$	1.6539	$K_2PdF_6$
0.8304	$BaMnO_3$	1.6564	$BP$
0.8539	$BaTiSe_3$	1.6599	$Rb_2TiF_6$
0.8567	$RbCoCl_3$	1.7151	$Ni_2Mo_3O_8$
0.8659	$BaNiO_3$	1.7172	$Mg_2Mo_3O_8$
0.8660	$BaTiS_3$	1.7193	$Co_2Mo_3O_8$
0.9412	$H_2O$	1.7196	$Zn_2Mo_3O_8$
1.5842	$Cs_3TiBr_6$	1.7265	$CdCsP_4O_{14} \cdot 6H_2O$
1.5878	$(Fe, V)_4V_6O_{16}$	1.7269	$CsMnP_4O_{14} \cdot 6H_2O$
1.5952	$CuH$	1.7273	$CsMgP_4O_{14} \cdot 6H_2O$
1.5965	$ZnO$	1.7375	$Fe_2Mo_3O_8$
1.5991	$NH_4F$	1.7717	$Mn_2Mo_3O_8$
1.5995	$AlN$	1.8535	$Cd_2Mo_3O_8$
1.6033	$Rb_3TiBr_6$	2.2765	$Ce_{24}Co_{11}$
1.6046	$Ag_2In_2S_4$	2.4099	$Na_2CaBa_4RE_{1.5}Sr_{0.2}U_{0.3}(CO_3)_9$
1.6105	$Cs_2RhF_6$	2.5602	$CaOHCl$
1.6111	$InN$	2.8060	$CdOHCl$
1.6177	$MnS$	3.0630	$PbI_2$
1.6195	$Al_2Se_3$	3.1521	$CdBr_2$
1.6212	$Rb_2GeF_6$	3.2241	$CdI_2$
1.6218	$GaN$	3.2601	$CSi$
1.6221	$Rb_2PdF_6$	3.2669	$ZnS$
1.6224	$BeO$	3.3237	$Ti_3S_4$
1.6227	$BeO$	3.3294	$Ti_2S_3$
1.6231	$BeO$	3.7009	$TaSe_2$
1.6231	$Rb_2MnF_6$	3.7048	$TaS_2$
1.6235	$K_2GeF_6$	4.9019	$ZnS$
1.6236	$Be_4NaSbO_7$	4.9058	$CSi$
1.6245	$GaN$	4.9778	$AgI$
1.6245	$(Cd_{0.542}Zn_{0.458})S$	6.5340	$ZnS$
1.6251	$(Cd_{0.576}Zn_{0.424})S$	6.5434	$CSi$
1.6272	$ZnFe_{0.5}Mn_{0.5}S_2$	6.6047	$Al_5C_3N$
1.6281	$(Zn_{0.584}Cd_{0.415})S$	8.1590	$ZnS$
1.6286	$Rb_2CrF_6$	9.8264	$Al_7C_3N_3$

## Organic

0.6596	$Fe_7C_3$	1.6409	$SiC$
0.7038	$SP(C_2H_5)_3$	1.711	$C(NH_2)_3I$
0.7220	$SeP(C_2H_5)_3$	3.260	$SiC$
0.8436	$(C_2H_5)_3NHCl$	4.906	$SiC$
0.875	$(C_2H_5)_3NHBr$	6.5434	$SiC$
0.882	$(C_2H_5)_3NHI$	6.6047	$Al_5C_3N$
1.4119	$(CH_3)_4AsBr$	9.8264	$Al_7C_3N_3$

$\bar{6} m 2$ $\bar{6} 2 m$	$P\bar{6}m2$	$D_{3h}^1$	No. 187	Inorganic - 23 Organic - 4
Inorganic				
0.9394	NbN <sub>0.86</sub>		1.9957	Co <sub>2</sub> N <sub>5</sub> Ta <sub>4</sub>
0.9681	Ti <sub>3</sub> S <sub>2</sub>		1.9956	Fe <sub>2</sub> N <sub>5.2</sub> Ta <sub>4</sub>
0.9759	CW		2.0046	N <sub>4.5</sub> Ni <sub>2</sub> Ta <sub>4</sub>
0.9766	TiS		2.4384	Co <sub>3</sub> V
0.9768	NW		2.9211	Be <sub>17</sub> Hf <sub>2</sub>
0.9832	N <sub>0.83</sub> Ta		2.9310	U <sub>2</sub> Zn <sub>17</sub>
0.9864	N(Ti,Co)		3.9359	RbSc <sub>2</sub>
0.9901	MoP		4.7816	Fe <sub>3</sub> Th
1.0186	Zr <sub>3</sub> Se <sub>2</sub>		4.8052	Zn <sub>3</sub> In <sub>2</sub> S <sub>6</sub>
1.0648	TaZrN <sub>2</sub>		5.6194	3CeFC <sub>3</sub> •2CaC <sub>2</sub>
1.1114	CeFC <sub>3</sub> •CaC <sub>2</sub>		7.4344	TaSe <sub>2</sub>
1.1836	CeFC <sub>3</sub>			
Organic				
0.9759	WC		1.1836	CeFC <sub>3</sub>
1.111	CeFC <sub>3</sub> •CaC <sub>2</sub>		5.619	3CeFC <sub>3</sub> •2CaC <sub>2</sub>

$\bar{6} m 2$ $\bar{6} 2 m$	$P\bar{6}c2$	$D_{3h}^2$	No. 188	Inorganic - 19 Organic - 0
Inorganic				
1.3529	YbB <sub>3</sub>		1.4758	CoK(P <sub>3</sub> ) <sub>3</sub>
1.4583	KNi(BeF <sub>3</sub> ) <sub>3</sub>		1.4765	BaTiGe <sub>3</sub> O <sub>9</sub>
1.4608	KMg(BeF <sub>3</sub> ) <sub>3</sub>		1.4795	KMg(P <sub>3</sub> ) <sub>3</sub>
1.4618	KZn(BeF <sub>3</sub> ) <sub>3</sub>		1.4834	CdTi(P <sub>3</sub> ) <sub>3</sub>
1.4634	BaTiSi <sub>3</sub> O <sub>9</sub>		1.4889	CdRb(P <sub>3</sub> ) <sub>3</sub>
1.4638	CoK(BeF <sub>3</sub> ) <sub>3</sub>		1.4894	KMn(P <sub>3</sub> ) <sub>3</sub>
1.4654	KMn(BeF <sub>3</sub> ) <sub>3</sub>		1.4968	CdK(P <sub>3</sub> ) <sub>3</sub>
1.4657	Ba(Sn,Ti)Si <sub>3</sub> O <sub>9</sub>		1.4982	CdAg(P <sub>3</sub> ) <sub>3</sub>
1.4712	BaTiSi <sub>3</sub> O <sub>9</sub>		1.5211	CaK(P <sub>3</sub> ) <sub>3</sub>
1.4749	KZn(P <sub>3</sub> ) <sub>3</sub>			

$\bar{6} m 2$ $\bar{6} 2 m$	$P\bar{6}2m$	$D_{3h}^3$	No. 189	Inorganic - 32 Organic - 1
Inorganic				
0.2490	Be <sub>12</sub> Ti		0.5773	Ni <sub>2</sub> P
0.3391	Ca <sub>2</sub> Ir <sub>2</sub> O <sub>4</sub>		0.5773	KCeF <sub>4</sub>
0.4138	InMg <sub>2</sub>		0.5773	K <sub>2</sub> UF <sub>6</sub>
0.4742	BNi <sub>6</sub> Si <sub>2</sub>		0.5804	K <sub>2</sub> UF <sub>6</sub>
0.5156	PTi <sub>2</sub>		0.5811	KLaF <sub>4</sub>
0.5284	GePt <sub>2</sub>		0.5811	K <sub>2</sub> ThF <sub>6</sub>
0.5285	Pd <sub>2</sub> Si		0.5864	AsCo <sub>2</sub>
0.5386	AsPd <sub>2</sub>		0.5876	Fe <sub>2</sub> P
0.5438	AsPd <sub>2</sub>		0.5893	Fe <sub>2</sub> P
0.5454	Pd <sub>5</sub> Th <sub>3</sub>		0.5901	Fe <sub>2</sub> P
0.5457	Pt <sub>5</sub> Th <sub>3</sub>		0.5988	K <sub>2</sub> ThF <sub>6</sub>
0.5545	Pt <sub>2</sub> Si		0.6849	(Ce,La)FC <sub>3</sub>
0.5591	Rh <sub>2</sub> ThF <sub>6</sub>		0.7186	Na <sub>2</sub> O <sub>2</sub>
0.5687	Mn <sub>2</sub> P		0.8694	Ba <sub>0.5</sub> Ta <sub>2</sub> O <sub>3</sub>
0.5733	K <sub>2</sub> ReH <sub>9</sub>		0.9020	TiI <sub>3</sub>
0.5768	K <sub>2</sub> TcH <sub>9</sub>		1.1964	Al <sub>8</sub> FeMg <sub>3</sub> Si <sub>6</sub>
Organic				
0.6849	(Ce,La)FC <sub>3</sub>			

$\bar{6} m 2$ $\bar{6} 2 m$	$P\bar{6}2c$	$D_{3h}^4$	No. 190	Inorganic - 10 Organic - 9
Inorganic				
0.5071	(AgNS <sub>2</sub> •H <sub>2</sub> O) <sub>3</sub>		0.8891	K <sub>3</sub> NaUO <sub>2</sub> (C <sub>2</sub> O <sub>3</sub> ) <sub>3</sub>
0.5374	Co(N <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> •3N <sub>2</sub> H <sub>4</sub>		1.3665	CeFC <sub>3</sub>
0.5433	Zn(N <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> •3N <sub>2</sub> H <sub>4</sub>		1.3710	(La,Ce)C <sub>2</sub> O <sub>3</sub> F
0.5615	Cd(N <sub>2</sub> O <sub>3</sub> ) <sub>2</sub> •3N <sub>2</sub> H <sub>4</sub>		1.9711	FeS
0.7956	LiNaC <sub>2</sub> O <sub>3</sub>		3.8521	Ti <sub>2</sub> S <sub>3</sub>

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 $P\bar{6}2c$   $D_{3h}^4$  No. 190 (continued)  
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## Organic

0.5573	$NaI \cdot 3(CH_3)_2NCH_3$	1.206	$(CH_3)_3SbBr_2$
0.6413	$Na_3C_6N_9 \cdot 3H_2O$	1.273	$(CH_3)_3SbI_2$
0.796	$LiNaC_6O_3$	1.3665	$CeFC_6O_3$
0.8891	$K_3NaU_6O_{12}(C_6O_3)_3$	1.3710	$(La, Ce)C_6O_3F$
1.161	$(CH_3)_3SbCl_2$		

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 $\frac{6}{m} \frac{2}{m} \frac{2}{m}$   
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$P6/mmm$   $D_{6h}^1$  No. 191

Inorganic - 220  
Organic - 3  
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## Inorganic

0.3152	$KAlSi_4$	0.7988	$Co_5Gd$
0.3355	$Co(ClO_4)_2 \cdot 6H_2O$	0.8002	$Co_5Y$
0.3851	$Fe_4(OH)_3(P_6O_4)_3 \cdot 12H_2O$	0.8008	$Ni_5Pr$
0.4923	$Be_3Al_2Si_6O_{18}$	0.8016	$Co_5Sm$
0.5118	$AsPd_3$	0.8022	$Cu_5Pr$
0.5608	$NTa$	0.8023	$NdNi_5$
0.5769	$TiO_{0.55}$	0.8024	$CaCu_5$
0.5887	$Tl_2Ge_7O_{15}$	0.8026	$Co_5Er$
0.5897	$TiU_2$	0.8027	$Ni_5Pr$
0.5986	$BiIn_2$	0.8037	$Cu_5Nd$
0.6123	$UZr_2$	0.8037	$Ce_{1.2}Cu_{4.8}$
0.6286	$Ag_{5-x}Te_3$	0.8038	$NdNi_5$
0.6286	$Ag_5Te_3$	0.8047	$Cu_5Nd$
0.6298	$Ag_7Te_4$	0.8053	$Co_5Gd$
0.6315	$Ag_5Te_3$	0.8053	$Ni_5Sm$
0.6467	$Hg_2U$	0.8066	$CoSn$
0.6677	$PtZn_{1.7}$	0.8068	$Ni_5Th$
0.6724	$Mn_2Ta_3$	0.8068	$Ir_5Th$
0.6932	$Ag_2Th$	0.8069	$GdNi_5$
0.7021	$Cd_2Th$	0.8074	$Au_5(Ba, Au)$
0.7039	$Cd_2Dy$	0.8078	$LaNi_5$
0.7177	$Au_2Th$	0.8086	$Co_5Dy$
0.7186	$ErHg_2$	0.8096	$Co_5Dy$
0.7212	$Hg_2Ho$	0.8097	$Cu_5Ho$
0.7212	$DyHg_2$	0.8099	$Ni_5Y$
0.7311	$CaHg_2$	0.8101	$Co_5Y$
0.7342	$Hg_2La$	0.8103	$Ni_5Y$
0.7455	$EuHg_2$	0.8108	$Ni_5Th$
0.7636	$Be_5Zr$	0.8110	$GdNi_5$
0.7655	$Be_5Hf$	0.8115	$Co_5Ho$
0.7694	$CeZn_5$	0.8115	$HoNi_5$
0.7715	$C_3Si_{16}U_{20}$	0.8120	$FeGe$
0.7722	$Au_5Rb$	0.8122	$Ag_5Ba$
0.7739	$CaZn_5$	0.8125	$LaPt_5$
0.7780	$Cu_5Sr$	0.8135	$Ni_5Y$
0.7784	$Co_5La$	0.8137	$DyNi_5$
0.7787	$LaZn_5$	0.8139	$Ag_5Sr$
0.7836	$Fe_5Th$	0.8140	$HoNi_5$
0.7849	$Hg_2Sr$	0.8144	$Ni_5Pu$
0.7857	$EuZn_5$	0.8152	$DyNi_5$
0.7887	$BaPt_5$	0.8158	$ErNi_5$
0.7895	$Cu_2Th$	0.8160	$Co_5Th$
0.7897	$CaZn_5$	0.8167	$ErNi_5$
0.7905	$Co_5Nd$	0.8167	$CePt_5$
0.7907	$BaPd_5$	0.8176	$DyNi_5$
0.7909	$Co_5Nd$	0.8180	$Co_5Dy$
0.7922	$Au_5K$	0.8180	$CeCo_5$
0.7924	$Co_5Th$	0.8191	$CeNi_5$
0.7932	$Cu_5La$	0.8191	$CeCo_5$
0.7933	$Co_5Pr$	0.8192	$Co_5Er$
0.7947	$LaNi_5$	0.8194	$PrPt_5$
0.7959	$Co_5Gd$	0.8200	$Fe_5Gd$
0.7960	$CaNi_5$	0.8204	$Cu_5Gd$
0.7963	$Cu_5La$	0.8215	$CeNi_5$
0.7964	$Co_5Pr$	0.8215	$NdPt_5$
0.7965	$CeCu_4$	0.8220	$NdPt_5$
0.7966	$Co_5Th$	0.8226	$CeNi_5$
0.7975	$CaCu_5$	0.8230	$CeFe_5$
0.7977	$Cu_2Th$	0.8236	$Cu_5Y$
0.7981	$Co_5Gd$	0.8260	$Cu_5Y$
0.7983	$CeCu_5$	0.8268	$ThZn_2$

P6/mmm  $D_{6h}^1$  No. 191 (continued)

## Inorganic (continued)

0.8277	PtTl	1.0485	(B, Be) <sub>2</sub> Hf
0.8277	Ag <sub>5</sub> Fu	1.0490	Ge <sub>3</sub> Tm <sub>2</sub>
0.8282	Co <sub>5</sub> Y	1.0495	B <sub>2</sub> Ta
0.8337	Fe <sub>5</sub> Y	1.0510	PuSi <sub>2</sub>
0.8363	Be <sub>2</sub> Hf	1.0514	Er <sub>2</sub> Ge <sub>3</sub>
0.8367	DyFe <sub>5</sub>	1.0532	Ge <sub>3</sub> Tb <sub>2</sub>
0.8367	Fe <sub>5</sub> Sm	1.0536	Dy <sub>2</sub> Ge <sub>3</sub>
0.8392	FeSn	1.0538	Ge <sub>3</sub> Ho <sub>2</sub>
0.8436	Fe <sub>5</sub> Ho	1.0544	Si <sub>2</sub> U
0.8440	FeSn	1.0556	Ge <sub>3</sub> Yb <sub>2</sub>
0.8451	YZn <sub>5</sub>	1.0574	Sc <sub>3</sub> Si <sub>5</sub>
0.8458	DyZn <sub>5</sub>	1.0574	Ge <sub>3</sub> Lu <sub>2</sub>
0.8481	Th <sub>0.6</sub> Zn <sub>5.4</sub>	1.0590	Si <sub>2</sub> Th
0.8711	C <sub>6</sub> Li	1.0598	Li <sub>3</sub> N
0.8760	Cu <sub>2</sub> La	1.0604	(B, Be) <sub>2</sub> Zr
0.9479	Al <sub>2</sub> Th	1.0608	B <sub>2</sub> Ta
0.9525	Ga <sub>2</sub> U	1.0617	B <sub>2</sub> Ti
0.9555	InNi	1.0653	B <sub>2</sub> Ti
0.9563	Si <sub>2</sub> U	1.0661	B <sub>2</sub> Ti
0.9599	ErGa <sub>2</sub>	1.0693	B <sub>2</sub> Nb
0.9610	(Mn, Sb, Ca) <sub>4</sub> (Mn, Fe, Mg) <sub>3</sub> [ $\sigma_8$ Si $\sigma_4$ ]	1.0713	B <sub>2</sub> Nb
0.9647	Ga <sub>2</sub> Ho	1.0731	DySi <sub>2-n</sub>
0.9676	Ga <sub>2</sub> Pu	1.0763	ErSi <sub>2</sub>
0.9677	DyGa <sub>2</sub>	1.0763	HoSi <sub>2-n</sub>
0.9678	Li <sub>2.32</sub> Co <sub>0.68</sub> N	1.0776	Si <sub>5</sub> Y <sub>3</sub>
0.9683	DyGa <sub>2</sub>	1.0777	Si <sub>2-n</sub> Tb
0.9693	CMo	1.0787	Si <sub>2-n</sub> Tm
0.9707	Ni <sub>2</sub> Th	1.0814	LuSi <sub>2-n</sub>
0.9707	Al <sub>2.12</sub> La <sub>0.88</sub>	1.0817	AlB <sub>2</sub>
0.9729	Ga <sub>2</sub> Tb	1.0867	Si <sub>2-n</sub> Yb
0.9755	Ga <sub>2</sub> Y	1.0893	Ga <sub>2</sub> Sr
0.9755	B <sub>2</sub> Be	1.1005	BaSi <sub>2</sub>
0.9765	Ga <sub>2</sub> Y	1.1047	B <sub>2</sub> Hf
0.9801	Ga <sub>2</sub> Gd	1.1139	B <sub>2</sub> Zr
0.9811	Ga <sub>2</sub> Gd	1.1145	B <sub>2</sub> Zr
0.9880	Ga <sub>2</sub> Sm	1.1179	B <sub>2</sub> Sc
0.9929	ThZn <sub>2</sub>	1.1346	DyGe <sub>1.62</sub>
0.9976	Si <sub>2</sub> Th	1.1411	B <sub>2</sub> Lu
1.0000	Ga <sub>2</sub> Nd	1.1420	B <sub>2</sub> Mg
1.0046	CeGa <sub>2</sub>	1.1426	BaGa <sub>2</sub>
1.0061	Ga <sub>2</sub> Pr	1.2717	B <sub>2</sub> U
1.0099	B <sub>2</sub> W	1.3604	Pt $\sigma_2$
1.0100	B <sub>2</sub> Mn	1.4933	BaAl <sub>2</sub> Si <sub>2</sub> $\sigma_8$
1.0131	B <sub>2</sub> Mo	1.6104	Fe <sub>2</sub> GaGe
1.0197	B <sub>2</sub> V	1.7053	KAs <sub>4</sub> $\sigma_6$ Br
1.0207	B <sub>2</sub> Mo	1.7168	Cu <sub>2</sub> Te
1.0222	Ga <sub>2</sub> La	1.7221	NaAs <sub>4</sub> $\sigma_6$ I
1.0356	EuGa <sub>2</sub>	1.7376	KAs <sub>4</sub> $\sigma_6$ I
1.0365	B <sub>2</sub> (Cr, Mo)	1.7633	NH <sub>4</sub> As <sub>4</sub> $\sigma_6$ I

## Organic

0.7715	U <sub>20</sub> Si <sub>16</sub> C <sub>3</sub>	0.9693	MoC
0.8711	LiC <sub>6</sub>		

$\begin{matrix} 6 & 2 & 2 \\ m & m & m \end{matrix}$

P6/mcc  $D_{6h}^2$  No. 192

Inorganic - 11  
Organic - 1

## Inorganic

0.9572	Mg <sub>2</sub> Al <sub>4</sub> Si <sub>5</sub> $\sigma_{18}$	1.0016	Be <sub>6-n/2</sub> (Na, Li, K, Cs) <sub>n</sub> Al <sub>4</sub> Si <sub>12</sub> $\sigma_{36}$ $\bullet n$ H <sub>2</sub> $\sigma$
0.9579	(Fe, Mg)(Sc, Al) <sub>3</sub> HSi <sub>6</sub> $\sigma_{18}$	1.3279	K <sub>2</sub> Ce <sub>4</sub> Be <sub>4</sub> Al <sub>2</sub> Si <sub>24</sub> $\sigma_{60}$ $\bullet$ H <sub>2</sub> $\sigma$
0.9663	[Be <sub>3</sub> Sc <sub>2</sub> Si <sub>6</sub> $\sigma_{18}$ ]	1.4094	(K, Na) <sub>2</sub> (Fe, Mg) <sub>5</sub> Si <sub>12</sub> $\sigma_{30}$
0.9957	Be <sub>3</sub> Al <sub>2</sub> Si <sub>6</sub> $\sigma_{18}$	1.4100	(K, Na, Ca)(MgFe) <sub>2</sub> (AlFeFe) <sub>3</sub> (Si, Al) <sub>12</sub> $\sigma_{30}$ $\bullet$ H <sub>2</sub> $\sigma$
0.9979	Be <sub>3</sub> Al <sub>2</sub> Si <sub>6</sub> $\sigma_{18}$	1.4208	(K, Na, Ca)(Mg, Fe) <sub>2</sub> [Al, Fe(II), Fe(III)] <sub>3</sub> (Si, Al) <sub>12</sub> $\sigma_{30}$ $\bullet$ H <sub>2</sub> $\sigma$
1.0001	Be <sub>3</sub> Al <sub>2</sub> Si <sub>6</sub> $\sigma_{18}$		

## Organic

0.3390	BrC <sub>6</sub> H <sub>4</sub> B( $\sigma$ H) <sub>2</sub>		
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$\frac{6}{m} \frac{2}{m} \frac{2}{m}$ 
 $P6_3/mcm$   $D_{6h}^3$  No. 193

 Inorganic - 97  
 Organic - 1

## Inorganic

0.6739	$Ga_3V_5\theta_x$	0.7308	$Nd_5Pb_3$
0.6752	$Ge_3U_5$	0.7312	$Gd_5Pb_3$
0.6757	$(Cr,C)_5(Si,C)_3$	0.7313	$Pb_3Tb_5$
0.6776	$Sn_3Ti_5$	0.7315	$Lu_5Sn_3$
0.6793	$Ge_3N_xTa_5$	0.7321	$Er_5Sn_3$
0.6800	$Ga_3Nb_5\theta_x$	0.7321	$Ho_5Pb_3$
0.6813	$Ge_3V_5$	0.7335	$Er_5Pb_3$
0.6816	$Al_3B_xTa_5$	0.7342	$Sn_3Y_5$
0.6832	$Sn_3Zr_5$	0.7345	$Pb_3Tm_5$
0.6849	$Hf_5Sn_3$	0.7356	$La_5Sn_3$
0.6867	$Si_3Ti_5$	0.7385	$Lu_5Pb_3$
0.6878	$Pb_3Zr_5$	0.7393	$Sc_5Si_3$
0.6886	$C_xGe_3Mo_5$	0.7403	$Ce_5Ge_3$
0.6898	$Ga_3N_xTa_5$	0.7410	$Ge_3Sc_5$
0.6900	$Ga_3N_xNb_5$	0.7488	$Ge_3Lu_5$
0.6905	$Ge_3Ta_5$	0.7491	$Ge_3Tb_5$
0.6918	$Si_3Ti_5$	0.7494	$Ce_5Ge_3$
0.6930	$Ge_3Ti_5$	0.7497	$Ge_3Tm_5$
0.6934	$Ge_3Zr_5$	0.7497	$Er_5Ge_3$
0.6940	$Hf_5Sn_3$	0.7500	$Ge_3Ho_5$
0.6964	$Nb_5Si_3$	0.7500	$Ge_3Nd_5$
0.6967	$Mn_5Si_3$	0.7500	$Ge_3Pr_5$
0.6968	$Nb_5Si_3$	0.7503	$Ge_3Sm_5$
0.6992	$Si_3Ta_5$	0.7506	$Dy_5Ge_3$
0.7002	$Ge_3Zr_5$	0.7518	$Gd_5Ge_3$
0.7024	$Ge_3Hf_5$	0.7522	$Ge_3La_5$
0.7029	$P_3Ti_5$	0.7585	$Ge_3La_5$
0.7033	$Ge_3Mn_5$	0.8565	$Cs_3\theta$
0.7036	$P_3Ti_5$	0.9121	$HfI_3$
0.7039	$Hf_5Al_3\theta_x$	0.9159	$ZrI_3$
0.7045	$Hf_5Si_3$	0.9229	$RuCl_3$
0.7047	$As_3Ti_5$	0.9282	$TiCl_3$
0.7048	$Si_3Zr_5$	0.9356	$ZrBr_3$
0.7066	$Ge_3N_xNb_5$	0.9402	$Al_2S_3$
0.7066	$C_xGe_3Nb_5$	0.9613	$ZrCl_3$
0.7067	$Al_3Hf_5$	0.9654	$ZrCl_3$
0.7109	$Al_3Zr_5$	1.0093	$BaUF_6$
0.7180	$Hg_3Mg_5$	1.0221	$HoF_3$
0.7272	$Pr_5Sn_3$	1.0235	$CeF_3$
0.7273	$Sm_5Sn_3$	1.0236	$SmF_3$
0.7282	$Gd_5Sn_3$	1.0244	$Rb_{0.29}W\theta_3$
0.7298	$Pb_3Sm_5$	1.0249	$NdF_3$
0.7298	$Pb_3Pr_5$	1.0253	$EuF_3$
0.7301	$Nd_5Sn_3$	1.0285	$CsW_3\theta_9$
0.7302	$Ho_5Sn_3$	1.0321	$K_{0.31}W\theta_3$
0.7302	$Dy_5Sn_3$	1.6311	$FeTiV$
0.7304	$Sn_3Tb_5$	1.7480	$BaUF_6$
0.7305	$Sn_3Tm_5$	2.8863	$CaAl_2Si_2\theta_8$
0.7308	$Dy_5Pb_3$		

## Organic

0.6757  $(Cr,C)_5(Si,C)_3$ 
 $\frac{6}{m} \frac{2}{m} \frac{2}{m}$ 
 $P6_3/mmc$   $D_{6h}^4$  No. 194

 Inorganic - 637  
 Organic - 48

## Inorganic

0.4180	$CaNa_3Al_3(Si\theta_4)_3S\theta_4$	0.7266	$Al_3Gd$
0.6023	$Nb_6Sn_5$	0.7275	$Al_3Gd$
0.6092	$Ga_5V_6$	0.7407	$Ba(Pb_{0.5}Tl_{0.5})_3$
0.6144	$Na_2R_4(C\theta_3)_5$	0.7411	$Hg_3Sr$
0.6171	$Sn_5Ti_6$	0.7418	$GdHg_3$
0.6682	$Cu_1\theta Cl_4(S\theta_4)(\theta R)_{32} \cdot 3H_2\theta$	0.7444	$Hg_3Tb$
0.6918	$Al_3La$	0.7445	$Hg_3Y$
0.7042	$Al_3Ce$	0.7462	$DyHg_3$
0.7079	$Al_3Pr$	0.7466	$Hg_3Ho$
0.7117	$Al_3Nd$	0.7468	$EuHg_3$
0.7118	$Al_3Th$	0.7476	$Hg_3Sc$
0.7170	$Al_6ThU$	0.7480	$ErHg_3$
0.7205	$Al_3Sm$	0.7481	$Hg_3Tm$

P6<sub>3</sub>/mmc D<sub>6h</sub><sup>4</sup> No. 194 (continued)

## Inorganic (continued)

0.7495	DyHg <sub>3</sub>	1.0471	Al <sub>10</sub> Mn <sub>3</sub>
0.7501	Hg <sub>3</sub> Lu	1.0694	SbCl <sub>5</sub>
0.7506	Hg <sub>3</sub> Ho	1.0896	SnTi <sub>2</sub>
0.7508	ErHg <sub>3</sub>	1.1872	[Co(NH <sub>3</sub> ) <sub>3</sub> H <sub>2</sub> OCl <sub>2</sub> ]Cl
0.7568	CaHg <sub>3</sub>	1.2083	BPt
0.7570	EuTi <sub>3</sub>	1.2114	AlZr <sub>2</sub>
0.7612	Hg <sub>3</sub> Yb	1.2195	GaTi <sub>2</sub>
0.7648	AlLa <sub>3</sub>	1.2220	N <sub>2</sub> O <sub>5</sub>
0.7760	AlNd <sub>3</sub>	1.2296	InNi
0.7974	InNi <sub>3</sub>	1.2309	Fe <sub>3</sub> Sn <sub>2</sub>
0.7990	Fe <sub>3</sub> Sn	1.2425	Mn <sub>2</sub> Sn
0.8007	AlTi <sub>3</sub>	1.2457	GaNi <sub>2</sub>
0.8026	Ni <sub>3</sub> Sn	1.2476	Fe <sub>3</sub> Ge <sub>2</sub>
0.8031	AlTi <sub>2</sub>	1.2529	Mn <sub>1.74</sub> Sn
0.8033	Ir <sub>5</sub> Th	1.2577	Ni <sub>3</sub> Sn <sub>2</sub>
0.8047	Co <sub>3</sub> W	1.2589	Co <sub>3</sub> Sn <sub>2</sub>
0.8051	SnTi <sub>3</sub>	1.2593	Co <sub>3</sub> Ge <sub>2</sub>
0.8053	SnTi <sub>3</sub>	1.2623	FeSb
0.8063	CsTiBr <sub>3</sub>	1.2636	Rh <sub>2</sub> Th
0.8070	SbTi <sub>4</sub>	1.2678	NiSn
0.8074	PbTi <sub>4</sub>	1.2683	Cu <sub>2</sub> Ni <sub>3</sub> Sn <sub>3</sub>
0.8093	Cd <sub>3</sub> Mg	1.2699	Ge <sub>2</sub> Ni <sub>3</sub>
0.8099	CdMg <sub>3</sub>	1.2750	AuSn
0.8150	RbTiBr <sub>3</sub>	1.2756	SbV
0.8209	Ni <sub>3</sub> (Ta <sub>0.33</sub> Ti <sub>0.67</sub> )	1.2779	AuSn
0.8209	Ni <sub>3</sub> (Nb <sub>0.33</sub> Ti <sub>0.67</sub> )	1.2800	[Rh <sub>3</sub> Sn <sub>2</sub> ]
0.8259	CsNiCl <sub>3</sub>	1.2850	Co <sub>2</sub> Ge
0.8379	CsNiF <sub>3</sub>	1.2880	Pd <sub>3</sub> Sn <sub>2</sub>
0.8499	Pt <sub>3</sub> U	1.2967	NiSb
0.8623	BaCoO <sub>2.85</sub>	1.3047	NiSb
0.9437	Cd <sub>3</sub> Mg	1.3078	NiSb
0.9502	Ni <sub>17</sub> Sm <sub>2</sub>	1.3208	CrSb
0.9547	Gd <sub>2</sub> Ni <sub>17</sub>	1.3229	PtSn
0.9639	Ni <sub>17</sub> Pu <sub>2</sub>	1.3242	CrSb
0.9670	Ni <sub>17</sub> Tb <sub>2</sub>	1.3249	PtSb
0.9673	Ho <sub>2</sub> Ni <sub>17</sub>	1.3314	CrSb
0.9674	Er <sub>2</sub> Ni <sub>17</sub>	1.3363	CoSb
0.9678	Ni <sub>17</sub> Y <sub>2</sub>	1.3420	CoSb
0.9684	Dy <sub>2</sub> Ni <sub>17</sub>	1.3495	BiMn
0.9690	Ce <sub>2</sub> Co <sub>17</sub>	1.3530	NiTe
0.9709	Co <sub>17</sub> Dy <sub>2</sub>	1.3541	Na <sub>2</sub> ZrSi <sub>3</sub> O <sub>9</sub> •2H <sub>2</sub> O
0.9715	Co <sub>17</sub> Gd <sub>2</sub>	1.3660	PdTe
0.9719	Ce <sub>2</sub> Co <sub>17</sub>	1.3705	IrTe
0.9721	Co <sub>17</sub> Y <sub>2</sub>	1.3763	BiMn
0.9725	Ni <sub>17</sub> Th <sub>2</sub>	1.3793	CoTe
0.9729	Co <sub>17</sub> Gd <sub>2</sub>	1.3807	CoTe
0.9732	Co <sub>17</sub> Sm <sub>2</sub>	1.3832	BiRh
0.9733	Co <sub>17</sub> Tb <sub>2</sub>	1.3879	IrSb
0.9741	Co <sub>17</sub> Y <sub>2</sub>	1.3880	BiRh
0.9743	Co <sub>17</sub> Ho <sub>2</sub>	1.3900	MnSb
0.9751	Co <sub>17</sub> Ho <sub>2</sub>	1.3910	AsNi
0.9756	Co <sub>17</sub> Dy <sub>2</sub>	1.3940	IrPb
0.9762	Fe <sub>17</sub> Y <sub>2</sub>	1.3960	IrSn
0.9763	Co <sub>17</sub> Er <sub>2</sub>	1.4029	MnSb
0.9769	Co <sub>17</sub> Er <sub>2</sub>	1.4152	AlPd
0.9799	Co <sub>17</sub> Tm <sub>2</sub>	1.4185	RhTe
0.9813	Fe <sub>17</sub> Tb <sub>2</sub>	1.4209	BiMn
0.9822	Fe <sub>17</sub> Ho <sub>2</sub>	1.4605	CoSe
0.9824	Fe <sub>17</sub> Gd <sub>2</sub>	1.4630	NiSe
0.9835	Er <sub>2</sub> Fe <sub>17</sub>	1.4681	CoSe
0.9838	Fe <sub>17</sub> Gd <sub>2</sub>	1.4760	Co <sub>3</sub> SiU <sub>2</sub>
0.9841	Dy <sub>2</sub> Fe <sub>17</sub>	1.4818	Fe <sub>2</sub> Te <sub>3</sub>
0.9858	Fe <sub>17</sub> Ho <sub>2</sub>	1.5000	Fe <sub>3</sub> SiU <sub>2</sub>
0.9884	La <sub>2</sub> Mg <sub>17</sub>	1.5023	AlCo <sub>3</sub> U <sub>2</sub>
0.9890	Al <sub>11</sub> C <sub>6</sub> Cu <sub>3</sub> Mo <sub>12</sub>	1.5063	RhSe
0.9918	Be <sub>17</sub> Ti <sub>2</sub>	1.5074	CoS
0.9918	Al <sub>5</sub> Co <sub>2</sub>	1.5266	CoS
0.9919	Be <sub>17</sub> Hf <sub>2</sub>	1.5302	Mn <sub>5</sub> Si <sub>3</sub> U <sub>4</sub>
0.9923	CeMg <sub>10.3</sub>	1.5340	AsMn
0.9954	Al <sub>5</sub> Rh <sub>2</sub>	1.5376	CoS
1.0000	C <sub>4</sub> Co <sub>3</sub> W <sub>9</sub>	1.5400	CoS
1.0185	Co <sub>17</sub> Sm <sub>2</sub>	1.5410	Cr <sub>1.33</sub> Te <sub>2</sub>
1.0308	Al <sub>9</sub> Mn <sub>3</sub> Si	1.5494	SbTi
1.0387	Al <sub>20</sub> Mn <sub>3.5</sub> Si <sub>1.1</sub> Zn <sub>1.4</sub>	1.5511	CoMoO <sub>6</sub>

P6<sub>3</sub>/mmc D<sub>6h</sub><sup>4</sup> No. 194 (continued)

## Inorganic (continued)

1.5541	NiS	1.6104	(Co,Ge) <sub>2</sub> Mo
1.5552	Cv <sub>2</sub>	1.6109	CdCu <sub>2</sub>
1.5578	NiS	1.6115	Co <sub>3</sub> GeNb <sub>2</sub>
1.5581	Cr <sub>2.00</sub> Te <sub>2</sub>	1.6127	Cr <sub>3</sub> SiU <sub>2</sub>
1.5600	CoW <sub>6</sub>	1.6129	Ga <sub>2</sub> Yb
1.5606	In <sub>2</sub> Yb	1.6130	FeMoSi
1.5673	FeW <sub>6</sub>	1.6131	Al <sub>0.6</sub> Co <sub>1.4</sub> Zr
1.5692	LuMn <sub>6</sub>	1.6137	Nd
1.5698	Ho	1.6138	NTa <sub>2</sub>
1.5700	Er	1.6142	Cr <sub>2</sub> Ti
1.5708	ScP <sub>6</sub> •2H <sub>2</sub> O	1.6143	Cu <sub>1.25</sub> Ga <sub>0.75</sub> Ti
1.5709	FeMo <sub>6</sub>	1.6148	Re
1.5709	Dy	1.6151	GaNb <sub>2</sub> Ni <sub>3</sub>
1.5722	Cu <sub>3</sub> Sn	1.6154	AlCoW
1.5723	Ge <sub>0.75</sub> MnNi <sub>1.25</sub>	1.6155	Co <sub>1.50</sub> Ga <sub>0.50</sub> Zr
1.5726	(Os, Ir, Rh, Pt, Ru, Fe)	1.6156	CrSe
1.5726	Cu <sub>3</sub> Sb	1.6156	KPh <sub>2</sub>
1.5762	Co <sub>1.1</sub> Si <sub>0.9</sub> V	1.6159	VRe <sub>6</sub>
1.5767	Cv <sub>2</sub>	1.6163	HaTl <sub>2</sub>
1.5768	Ga <sub>0.75</sub> MgNi <sub>1.25</sub>	1.6167	EuMg <sub>2</sub>
1.5772	Al <sub>3</sub> OsU <sub>2</sub>	1.6175	Co <sub>3</sub> GaTa <sub>2</sub>
1.5779	(Al, Mn) <sub>2</sub> U	1.6180	AlNiTa
1.5811	Hf	1.6182	FeSiW
1.5817	EuIn <sub>2</sub>	1.6186	AlNbNi
1.5817	EuTl <sub>2</sub>	1.6187	Co <sub>3</sub> Nb <sub>2</sub> Si
1.5819	Cv <sub>2</sub>	1.6194	SrTl <sub>2</sub>
1.5820	Ru	1.6199	Pr
1.5831	Os	1.6201	Cu <sub>1.25</sub> Ga <sub>0.75</sub> Mn
1.5832	CaIn <sub>2</sub>	1.6202	Cu <sub>5</sub> Ge
1.5836	Mn <sub>6</sub>	1.6202	Fe <sub>4.75</sub> Se <sub>52.5</sub>
1.5837	Ni <sub>1.2</sub> Si <sub>0.8</sub> V	1.6202	VSe
1.5845	Y	1.6207	Co <sub>3</sub> GaNb <sub>2</sub>
1.5847	Be	1.6212	TiZn <sub>2</sub>
1.5855	Ru	1.6216	AsCu <sub>4.5</sub>
1.5872	Y	1.6224	Mg <sub>2</sub> Yb
1.5879	Cu <sub>1.5</sub> Ge <sub>0.5</sub> Mg	1.6228	Co
1.5884	Sc	1.6232	Mn <sub>2</sub> Nd
1.5899	(Os, Ir)	1.6236	Mg
1.5900	CNb <sub>2</sub>	1.6238	CaMg <sub>2</sub>
1.5910	Gd	1.6240	Fe <sub>2</sub> Ti
1.5925	Zr	1.6243	NNb <sub>2</sub>
1.5926	CrRh	1.6250	Ni <sub>3</sub> Ti
1.5936	Sc	1.6253	CrSe
1.5949	Fe <sub>2/3</sub> N <sub>1/3</sub>	1.6256	Co <sub>2</sub> Nb
1.5955	Cu <sub>1.5</sub> Ge <sub>0.5</sub> Mn	1.6258	AlCuHf
1.5956	CoMoSi	1.6260	FeSe
1.5958	CuInMn	1.6260	Be <sub>2</sub> V
1.5962	Al <sub>2</sub> C <sub>6</sub>	1.6261	Cr
1.5973	MoNiSi	1.6268	Cr <sub>2</sub> Zr
1.5974	Tl	1.6270	Be <sub>2</sub> Fe
1.5975	(Ge, Ni) <sub>2</sub> Mo	1.6271	FeSe
1.5981	Mo <sub>5</sub> Si <sub>3</sub> U <sub>4</sub>	1.6271	Al <sub>0.75</sub> Fe <sub>1.25</sub> Zr
1.5982	Rh <sub>80.8</sub> W <sub>19.2</sub>	1.6272	Fe <sub>1.5</sub> Ga <sub>0.5</sub> Zr
1.5984	Tl	1.6273	FeGeMo
1.6000	LaTl <sub>3</sub>	1.6288	AlFeTa
1.6000	Tl	1.6289	H <sub>2</sub> O
1.6006	NiSiW	1.6295	Ni <sub>3</sub> Ti
1.6013	AlMnU	1.6298	Fe <sub>2</sub> W
1.6014	Ti	1.6298	Mg <sub>2</sub> Sr
1.6035	Co <sub>3</sub> GeTa <sub>2</sub>	1.6304	CoMgNi
1.6041	Tc	1.6309	CoCrNb
1.6042	In <sub>2</sub> Sr	1.6309	AlVZr
1.6056	BaMg <sub>2</sub>	1.6311	Be <sub>2</sub> Re
1.6057	Fe <sub>2</sub> Sc	1.6312	CoSiW
1.6063	Re <sub>2</sub> U	1.6316	Co <sub>2</sub> Ta
1.6070	AlNiTa	1.6316	Fe <sub>2</sub> Nb
1.6078	Ti <sub>6</sub> O <sub>325</sub>	1.6320	H <sub>2</sub>
1.6078	CoGaHf	1.6322	Be <sub>2</sub> Cr
1.6081	AlCoV	1.6326	Mn <sub>2</sub> Ta
1.6082	VTe	1.6328	AlHfMo
1.6086	Mg <sub>2</sub> Y	1.6328	Mn <sub>2</sub> Pr
1.6087	AlCuNb	1.6329	Be <sub>2</sub> Mn
1.6098	MgZn	1.6329	Cr <sub>2</sub> Zr
1.6102	CuGaNb	1.6331	He

P6<sub>3</sub>/mmc D<sub>6h</sub><sup>4</sup> No. 194 (continued)

## Inorganic (continued)

1.6331	Fe <sub>2</sub> Tl	1.6567	Os <sub>2</sub> Y
1.6331	HfOs <sub>2</sub>	1.6581	Re <sub>2</sub> Th
1.6332	Re <sub>2</sub> Zr	1.6587	FeS
1.6332	Mn <sub>2</sub> Th	1.6600	Fe <sub>1.74</sub> S <sub>2</sub>
1.6332	Hg <sub>2</sub> N <sub>2</sub> O <sub>2</sub> H <sub>2</sub> O	1.6602	Ru <sub>2</sub> Sc
1.6333	Fe <sub>2</sub> Ta	1.6611	Ba <sub>5/6</sub> Sr <sub>1/6</sub> Ru <sub>3</sub>
1.6335	HfOs <sub>2</sub>	1.6616	GdOs <sub>2</sub>
1.6337	Na	1.6617	Ni <sub>2</sub> U
1.6338	(Ti <sub>21</sub> Mo <sub>9</sub> )(Fe <sub>50</sub> Cr <sub>5</sub> Si <sub>5</sub> )	1.6622	Al <sub>2</sub> Zr
1.6340	ScTe	1.6628	NdOs <sub>2</sub>
1.6340	ErMn <sub>2</sub>	1.6640	Os <sub>2</sub> Sm
1.6342	Si <sub>2</sub>	1.6664	Os <sub>2</sub> Pr
1.6343	Sr	1.6667	TiTe
1.6344	Re <sub>2</sub> Y	1.6687	Ru <sub>2</sub> Sc
1.6345	Mn <sub>2</sub> Tm	1.6696	VSe
1.6345	Pt <sub>3</sub> Zr	1.6710	Pd <sub>3</sub> U
1.6348	LuMn <sub>2</sub>	1.6728	Ru <sub>2</sub> Y
1.6349	AlCuSc	1.6736	Pd <sub>3</sub> U
1.6351	Mn <sub>2</sub> Nb	1.6766	LuRu <sub>2</sub>
1.6351	Mn <sub>2</sub> Zr	1.6776	Fe <sub>1.92</sub> S <sub>2</sub>
1.6354	Mn <sub>2</sub> Ta	1.6779	Pd <sub>3</sub> Th
1.6357	Re <sub>2</sub> Y	1.6791	ErRu <sub>2</sub>
1.6358	CrNiNb	1.6815	ZrTe
1.6362	Pd <sub>3</sub> Ti	1.6833	Ru <sub>2</sub> Y
1.6364	CrGeNb	1.6892	GdRu <sub>2</sub>
1.6370	Cr <sub>2</sub> Ta	1.6896	FeS
1.6371	Li	1.6896	AsTi
1.6372	HfRe <sub>2</sub>	1.6932	Hg <sub>2</sub> NBr
1.6373	CaLi <sub>2</sub>	1.6970	Cu <sub>2</sub> S
1.6375	HfRe <sub>2</sub>	1.7013	Hg <sub>2</sub> Ni
1.6377	(Cr,Fe) <sub>2</sub> Ti	1.7069	FeS
1.6382	Ca	1.7097	Tc <sub>2</sub> Th
1.6382	Os <sub>2</sub> Sc	1.7114	Ba <sub>2/3</sub> Sr <sub>1/3</sub> Ir <sub>3</sub>
1.6383	Mn <sub>2</sub> Ti	1.7172	Cu <sub>2</sub> S
1.6385	HfRe <sub>2</sub>	1.7320	VS
1.6386	V <sub>2</sub> Zr	1.7568	BaThF <sub>6</sub>
1.6389	Be <sub>2</sub> Cr	1.7576	PbUF <sub>6</sub>
1.6394	Be <sub>2</sub> W	1.7640	AcF <sub>3</sub>
1.6396	GeTa <sub>2</sub> V <sub>3</sub>	1.7643	PbThF <sub>6</sub>
1.6403	KNa <sub>2</sub>	1.7653	AsNa <sub>3</sub>
1.6405	AlCuMg	1.7659	K <sub>3</sub> P
1.6407	Be <sub>2</sub> Mo	1.7665	Na <sub>3</sub> P
1.6409	Mn <sub>2</sub> Ti	1.7675	Li <sub>3</sub> Sb
1.6420	Au-Cd	1.7679	AsK <sub>3</sub>
1.6421	Fe <sub>1-x</sub> S	1.7697	BiK <sub>3</sub>
1.6430	Os <sub>2</sub> Zr	1.7707	NpF <sub>3</sub>
1.6434	CuGaMg	1.7714	PuF <sub>3</sub>
1.6437	Hg <sub>2</sub> N <sub>2</sub> O <sub>2</sub> H <sub>2</sub> O	1.7722	BiNa <sub>3</sub>
1.6441	MgZn <sub>2</sub>	1.7723	UF <sub>3</sub>
1.6447	Mn <sub>2</sub> Sc	1.7729	LaF <sub>3</sub>
1.6451	Tc <sub>2</sub> Tm	1.7733	Na <sub>3</sub> Sb
1.6452	TbTc <sub>2</sub>	1.7736	AsRb <sub>3</sub>
1.6459	DyTc <sub>2</sub>	1.7748	K <sub>3</sub> Sb
1.6459	GdTc <sub>2</sub>	1.7755	AmF <sub>3</sub>
1.6461	LuTc <sub>2</sub>	1.7758	Rb <sub>3</sub> Sb
1.6464	ErTc <sub>2</sub>	1.7764	SrThF <sub>6</sub>
1.6464	HoTc <sub>2</sub>	1.7765	CmF <sub>3</sub>
1.6466	Tc <sub>2</sub> Y	1.7765	AmF <sub>3</sub>
1.6471	Cr <sub>2</sub> Nb	1.7769	SrUF <sub>6</sub>
1.6472	Sr	1.7774	Li <sub>3</sub> P
1.6483	CrS	1.7781	HgMg <sub>3</sub>
1.6485	LuOs <sub>2</sub>	1.7803	AsLi <sub>3</sub>
1.6505	MgZn <sub>2</sub>	1.7803	Rb <sub>3</sub> Sb
1.6508	Au <sub>2</sub> Cd	1.7825	CaThF <sub>6</sub>
1.6514	N <sub>2</sub>	1.7850	BiRb <sub>3</sub>
1.6520	SiTa <sub>2</sub> V <sub>3</sub>	1.7924	SmH <sub>3</sub>
1.6537	BaMn <sub>3</sub>	1.7935	Bi <sub>0.1</sub> F <sub>2.8</sub>
1.6541	Al <sub>2</sub> Hf	1.7995	TbH <sub>3</sub>
1.6546	Ru <sub>2</sub> Zr	1.8012	HoH <sub>3</sub>
1.6555	Os <sub>2</sub> Y	1.8020	DyH <sub>3</sub>
1.6559	CrGaNb	1.8023	ErH <sub>3</sub>
1.6560	Be <sub>2</sub> Mo	1.8030	TmH <sub>3</sub>
1.6561	Al <sub>2</sub> Zr	1.8050	Th <sub>2</sub> F <sub>2</sub>
1.6564	Re <sub>2</sub> Th	1.8108	LuH <sub>3</sub>

P6<sub>3</sub>/mmc D<sub>6h</sub><sup>4</sup> No. 194 (continued)

## Inorganic (continued)

1.8135	YH <sub>3</sub>	3.3684	AsHf
1.8182	Mg <sub>3</sub> Pt	3.3699	AsTi
1.8233	AuMg <sub>3</sub>	3.3833	AsZr
1.8549	Zn	3.3890	HfP
1.8649	NbN <sub>0.95</sub>	3.4049	PZr
1.8852	Cd	3.4701	MnN <sub>4</sub> Ta <sub>3</sub>
1.8860	6Ca(θH) <sub>2</sub> •Al <sub>2</sub> (Crθ <sub>4</sub> ) <sub>3</sub> •24H <sub>2</sub> θ	3.4891	C <sub>2</sub> S <sub>2</sub> Ti <sub>4</sub>
1.9053	KAmθ <sub>2</sub> Cθ <sub>3</sub>	3.5632	Hf <sub>2</sub> FeC <sub>2</sub> S
1.9084	Al <sub>2</sub> Ca <sub>6</sub> (θH) <sub>12</sub> (Sθ <sub>4</sub> ) <sub>3</sub> •26H <sub>2</sub> θ	3.5660	C <sub>2</sub> S <sub>2</sub> Zr <sub>4</sub>
1.9141	B <sub>2</sub> H <sub>6</sub>	3.5921	NbS <sub>2</sub>
1.9312	KPuθ <sub>2</sub> Cθ <sub>3</sub>	3.6348	NbSe <sub>2</sub>
1.9322	BeHfSi	3.7055	TaSe <sub>2</sub>
1.9339	TiS	3.7215	TaSe
1.9380	BeZrSi	3.7415	CMo
1.9458	NbS	3.7855	Nb <sub>1+x</sub> S <sub>2</sub>
1.9475	KNpθ <sub>2</sub> Cθ <sub>3</sub>	3.7911	NbSe
1.9515	TiS	3.8062	N <sub>4</sub> W <sub>2.56</sub>
1.9560	PV	3.8110	NNb
2.0073	KU <sub>6</sub> F <sub>25</sub>	3.8978	WS <sub>2</sub>
2.0168	KTh <sub>6</sub> F <sub>25</sub>	3.8991	Cu <sub>0.65</sub> NbSe <sub>2</sub>
2.0300	CsU <sub>6</sub> F <sub>25</sub>	3.9033	WS <sub>2</sub>
2.0413	NH <sub>4</sub> Puθ <sub>2</sub> Cθ <sub>3</sub>	3.9048	MoS <sub>2</sub>
2.0430	RbAmθ <sub>2</sub> Cθ <sub>3</sub>	3.9150	Pb(Fe,Mn,Al,Ti) <sub>12</sub> θ <sub>19</sub>
2.1301	Al-Fe-Si	3.9161	Mo <sub>0.84</sub> N
2.2151	Al <sub>23</sub> V <sub>4</sub>	3.9170	PbFe <sub>12</sub> θ <sub>19</sub>
2.2522	CsAmθ <sub>2</sub> Cθ <sub>3</sub>	3.9194	Cu <sub>0.65</sub> NbS <sub>2</sub>
2.3689	Al <sub>3</sub> Pu	3.9195	WS <sub>2</sub>
2.3715	CaCθ <sub>3</sub>	3.9216	MoSe <sub>2</sub>
2.4216	BaFeθ <sub>3</sub>	3.9234	MoSe <sub>2</sub>
2.4262	CsMnF <sub>3</sub>	3.9249	SrFe <sub>12</sub> θ <sub>19</sub>
2.4401	BaFeθ <sub>3</sub>	3.9359	BaFe <sub>12</sub> θ <sub>19</sub>
2.4420	Cs <sub>3</sub> Ti <sub>2</sub> Br <sub>9</sub>	3.9422	WSe <sub>2</sub>
2.4491	RbNIF <sub>3</sub>	3.9423	CaAl <sub>12</sub> θ <sub>19</sub>
2.4499	BaTiθ <sub>3</sub>	3.9456	BaFe <sub>12</sub> θ <sub>19</sub>
2.4549	BaRu <sub>2/3</sub> Mg <sub>1/3</sub> θ <sub>3</sub>	3.9482	WSe <sub>2</sub>
2.4549	Cs <sub>3</sub> Ti <sub>2</sub> Cl <sub>9</sub>	3.9491	SrAl <sub>12</sub> θ <sub>19</sub>
2.4557	BaRu <sub>2/3</sub> Ni <sub>1/3</sub> θ <sub>3</sub>	3.9501	CaAl <sub>12</sub> θ <sub>19</sub>
2.4571	Ba(Ti <sub>0.75</sub> Pt <sub>0.25</sub> )θ <sub>3</sub>	3.9606	PbAl <sub>12</sub> θ <sub>19</sub>
2.4779	Cs <sub>3</sub> V <sub>2</sub> Cl <sub>9</sub>	3.9615	PbGa <sub>12</sub> θ <sub>19</sub>
2.4791	CsCdCl <sub>3</sub>	3.9718	MoTe <sub>2</sub>
2.4811	Rb <sub>3</sub> Ti <sub>2</sub> Br <sub>9</sub>	4.0033	KFe <sub>11</sub> θ <sub>17</sub>
2.4834	Cs <sub>3</sub> Cr <sub>2</sub> Cl <sub>9</sub>	4.0204	Al <sub>22</sub> Na <sub>2</sub> θ <sub>34</sub>
2.5121	Mg <sub>3</sub> Fe(θH) <sub>9</sub> •3H <sub>2</sub> θ	4.0287	Rb <sub>2</sub> Fe <sub>22</sub> θ <sub>34</sub>
2.5771	B <sub>2</sub> Tc	4.0558	Al <sub>2</sub> θ <sub>3</sub>
2.5786	B <sub>2</sub> Re	4.0598	Al <sub>22</sub> K <sub>2</sub> θ <sub>34</sub>
2.6602	BN	4.0649	Al <sub>12</sub> Baθ <sub>19</sub>
2.7251	C	4.0820	CGeV <sub>2</sub>
2.7979	EuAlθ <sub>3</sub>	4.0894	CCr <sub>2</sub> Ge
2.8177	GdAlθ <sub>3</sub>	4.1802	InSe
2.8329	TbAlθ <sub>3</sub>	4.1994	CGeTi <sub>2</sub>
2.8378	DyAlθ <sub>3</sub>	4.2453	GaSe
2.8587	YAlθ <sub>3</sub>	4.2781	CSnTi <sub>2</sub>
2.8638	HoAlθ <sub>3</sub>	4.3091	CHf <sub>2</sub> Pb
2.8689	ErAlθ <sub>3</sub>	4.3164	Ag <sub>0.7</sub> NbS <sub>2</sub>
2.9905	Pt <sub>2</sub> Sn <sub>3</sub>	4.3214	CuS
3.2252	La	4.3236	GaS
3.2271	Mg <sub>2</sub> Th	4.3325	CGaNb <sub>2</sub>
3.2317	NbZn <sub>2</sub>	4.3351	CPbZr <sub>2</sub>
3.2346	CdCu <sub>2</sub>	4.3424	CGaTi <sub>2</sub>
3.2391	Ce	4.3448	CHf <sub>2</sub> Sn
3.2411	Am	4.3591	CSnZr <sub>2</sub>
3.2543	HfZn <sub>2</sub>	4.3686	CGaMo <sub>2</sub>
3.2553	Fe <sub>2</sub> Zr	4.3695	CuSe
3.2590	Ni <sub>3</sub> Ti	4.3703	CGaV <sub>2</sub>
3.2592	Co <sub>2</sub> Ta	4.3714	CCr <sub>2</sub> Ga
3.2598	Co <sub>2</sub> Ti	4.3782	CuSe
3.2628	Co <sub>2</sub> Nb	4.3979	CTLZr <sub>2</sub>
3.2739	Fe <sub>2</sub> Sc	4.4040	CHf <sub>2</sub> Tl
3.2809	Co <sub>2</sub> Ta	4.4274	GaNi <sub>2</sub>
3.2820	MgNi <sub>2</sub>	4.4455	(Ce,La,Nd)FCθ <sub>3</sub> •CaCθ <sub>3</sub>
3.2952	Li <sub>0.25</sub> MgZn <sub>1.75</sub>	4.4542	CHf <sub>2</sub> In
3.3213	CeNi <sub>3</sub>	4.4547	CInZr <sub>2</sub>
3.3343	Ti <sub>3</sub> S <sub>4</sub>	4.4570	ALCNb <sub>2</sub>
3.3410	PTI	4.4737	ALCTi <sub>2</sub>

P6<sub>3</sub>/mmc D<sub>6h</sub><sup>4</sup> No. 194 (continued)

## Inorganic (continued)

4.4825	AlCCr <sub>2</sub>	4.9237	Ce <sub>2</sub> Ni <sub>7</sub>
4.4891	Ti <sub>2</sub> InC	5.0145	[Mg <sub>6</sub> Fe <sub>2</sub> (OH) <sub>16</sub> ](C <sub>6</sub> O <sub>3</sub> •4H <sub>2</sub> O)
4.4976	AlCTa <sub>2</sub>	5.0489	[Mg <sub>7</sub> Al <sub>4</sub> (OH) <sub>22</sub> ](Cl <sub>4</sub> •4H <sub>2</sub> O)
4.5108	AlCV <sub>2</sub>	5.2941	Ni <sub>0.87</sub> W
4.5285	InNZr <sub>2</sub>	5.5850	BaFe <sub>18</sub> O <sub>27</sub>
4.5458	AlNTi <sub>2</sub>	6.8222	2(Ce, La, Nd)FCO <sub>3</sub> •CaCO <sub>3</sub>
4.5462	InNTi <sub>2</sub>	7.2775	TaSe <sub>2</sub>
4.6499	CCdTi <sub>2</sub>	7.3242	NbSe <sub>2</sub>
4.6512	B <sub>5</sub> W <sub>2</sub>	28.6735	Ba <sub>11</sub> (Mn, Zn) <sub>10</sub> Fe <sub>72</sub> O <sub>129</sub>
4.8538	CMo		

## Organic

0.6144	Na <sub>2</sub> R <sub>4</sub> (C <sub>6</sub> O <sub>3</sub> ) <sub>5</sub>	4.332	Nb <sub>2</sub> GaC
0.6390	SrCN <sub>2</sub>	4.333	Zr <sub>2</sub> PbC
0.9890	Mo <sub>12</sub> Cu <sub>3</sub> Al <sub>11</sub> C <sub>6</sub>	4.342	Ti <sub>2</sub> GaC
1.0000	Co <sub>3</sub> W <sub>9</sub> C <sub>4</sub>	4.344	Hf <sub>2</sub> SnC
1.5278	C <sub>18</sub> H <sub>24</sub>	4.359	Zr <sub>2</sub> SnC
1.5767	V <sub>2</sub> C	4.369	Mo <sub>2</sub> GaC
1.5962	Al <sub>2</sub> C <sub>6</sub>	4.370	Cr <sub>2</sub> GaC
1.9053	KAm <sub>2</sub> C <sub>6</sub> O <sub>3</sub>	4.370	V <sub>2</sub> GaC
1.9312	KPu <sub>2</sub> C <sub>6</sub> O <sub>3</sub>	4.398	Zr <sub>2</sub> TlC
1.9475	KNp <sub>2</sub> C <sub>6</sub> O <sub>3</sub>	4.403	Hf <sub>2</sub> TlC
2.0413	NH <sub>4</sub> Pu <sub>2</sub> C <sub>6</sub> O <sub>3</sub>	4.446	(Ce, La, Nd)FCO <sub>3</sub> •CaCO <sub>3</sub>
2.0430	RbAm <sub>2</sub> C <sub>6</sub> O <sub>3</sub>	4.455	Hf <sub>2</sub> InC
2.2522	CsAm <sub>2</sub> C <sub>6</sub> O <sub>3</sub>	4.455	Zr <sub>2</sub> InC
2.3715	CaCO <sub>3</sub>	4.464	Nb <sub>2</sub> AlC
2.725	C	4.47	Ti <sub>2</sub> AlC
3.489	C <sub>2</sub> S <sub>2</sub> Ti <sub>4</sub>	4.483	Cr <sub>2</sub> AlC
3.5632	Hf <sub>2</sub> FeC <sub>2</sub> S	4.490	Ti <sub>2</sub> InC
3.566	C <sub>2</sub> S <sub>2</sub> Zr <sub>4</sub>	4.498	Ta <sub>2</sub> AlC
3.742	MoC	4.511	V <sub>2</sub> AlC
4.083	V <sub>2</sub> GeC	4.653	Ti <sub>2</sub> CdC
4.091	Cr <sub>2</sub> GeC	4.8538	MoC
4.199	Ti <sub>2</sub> GeC	4.854	MoC
4.278	Ti <sub>2</sub> SnC	5.759	Ti <sub>3</sub> SiC <sub>2</sub>
4.308	Hf <sub>2</sub> PbC	6.822	2(Ce, La, Nd)FCO <sub>3</sub> •CaCO <sub>3</sub>

2 3

P23 T<sup>1</sup> No. 195Inorganic - 5  
Organic - 2

## Inorganic

10.27	NaTi <sub>2</sub> Co(N <sub>2</sub> ) <sub>6</sub>	10.57	K <sub>2</sub> PbNi(N <sub>2</sub> ) <sub>6</sub>
10.37	N <sub>2</sub> H <sub>6</sub> NaCo(N <sub>2</sub> ) <sub>6</sub>	10.72	Cs <sub>2</sub> NaCo(N <sub>2</sub> ) <sub>6</sub>
10.41	NaRb <sub>2</sub> Co(N <sub>2</sub> ) <sub>6</sub>		

## Organic

8.78	C <sub>6</sub> H <sub>12</sub>	9.87	(CH <sub>3</sub> ) <sub>4</sub> Si <sub>6</sub> O <sub>4</sub>
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2 3

F23 T<sup>2</sup> No. 196Inorganic - 10  
Organic - 0

## Inorganic

7.78	KPF <sub>6</sub>	10.47	PbRbCo(N <sub>2</sub> ) <sub>6</sub>
7.94	NH <sub>4</sub> PF <sub>6</sub>	10.64	AgCs <sub>2</sub> Co(N <sub>2</sub> ) <sub>6</sub>
10.36	KPbCo(N <sub>2</sub> ) <sub>6</sub>	10.87	CsPbCo(N <sub>2</sub> ) <sub>6</sub>
10.40	NH <sub>4</sub> PbCo(N <sub>2</sub> ) <sub>6</sub>	18.75	Li <sub>22</sub> Si <sub>15</sub>
10.45	PbTlCo(N <sub>2</sub> ) <sub>6</sub>	20.08	Li <sub>22</sub> Pb <sub>5</sub>

## Organic

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2 3	I23 T <sup>3</sup>	No. 197	Inorganic - 7 Organic - 1
Inorganic			
8.429	Li <sub>3</sub> Nb $\sigma$ <sub>4</sub>	10.18	Fe <sub>2</sub> Bi <sub>24</sub> $\sigma$ <sub>39</sub>
10.10	SiBi <sub>12</sub> $\sigma$ <sub>20</sub>	10.25	PbBi <sub>12</sub> $\sigma$ <sub>20</sub>
10.11	Bi <sub>2</sub> $\sigma$ <sub>3</sub>	13.44	(NH <sub>4</sub> ) <sub>2</sub> [Ni(NH <sub>3</sub> ) <sub>2</sub> (CNS) <sub>4</sub> ] $\bullet$ H <sub>2</sub> $\sigma$
10.16	Al <sub>2</sub> Bi <sub>24</sub> $\sigma$ <sub>39</sub>		
Organic			
13.44	(NH <sub>4</sub> ) <sub>2</sub> [Ni(NH <sub>3</sub> ) <sub>2</sub> (CNS) <sub>4</sub> ] $\bullet$ H <sub>2</sub> $\sigma$		

2 3	P2 <sub>1</sub> 3 T <sup>4</sup>	No. 198	Inorganic - 80 Organic - 19
Inorganic			
4.446	NiSi	8.192	Li <sub>2</sub> ZnMn <sub>3</sub> $\sigma$ <sub>8</sub>
4.447	CoSi	8.339	Fe <sub>2</sub> $\sigma$ <sub>3</sub>
4.487	FeSi	8.627	(As <sub>4</sub> Te)(NO <sub>3</sub> ) <sub>2</sub>
4.557	MnSi	9.23	BiBr <sub>3</sub>
4.56	AlNi <sub>2</sub> Si	9.236	Hg <sub>3</sub> $\sigma$ Cl <sub>4</sub>
4.607	CrSi	9.611	Sr(Mn $\sigma$ <sub>4</sub> ) <sub>2</sub> $\bullet$ 3H <sub>2</sub> $\sigma$
4.629	CrSi	9.838	K <sub>2</sub> Ni <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
4.668	AuBe	9.904	(NH <sub>4</sub> ) <sub>2</sub> Ni <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
4.675	RhSi	9.920	K <sub>2</sub> Mg <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
4.775	ReSi	9.925	K <sub>2</sub> Zn <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
4.82	Al <sub>3</sub> Pd <sub>4</sub> Si	9.929	Co <sub>2</sub> K <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
4.866	AlPt	9.930	Ni <sub>2</sub> Rb <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
4.868	AlPd	9.979	Mg <sub>2</sub> (NH <sub>4</sub> ) <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
4.88	GaPd	9.997	Co <sub>2</sub> (NH <sub>4</sub> ) <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
4.90	GaPt	10.005	Mg <sub>2</sub> Rb <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.091	ND <sub>3</sub>	10.007	Fe <sub>2</sub> K <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.130	RhSn	10.024	K <sub>2</sub> Mn <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.138	NH <sub>3</sub>	10.026	Co <sub>2</sub> Rb <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.20	NH <sub>3</sub>	10.033	Co <sub>2</sub> Tl <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.22	HgPd	10.068	Fe <sub>2</sub> (NH <sub>4</sub> ) <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.51	Li <sub>3</sub> N	10.098	Fe <sub>2</sub> Rb <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.64	C $\sigma$	10.108	Fe <sub>2</sub> Tl <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.667	N <sub>2</sub>	10.114	K <sub>2</sub> Mn <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.68	NiAsS	10.192	(NH <sub>4</sub> ) <sub>2</sub> Mn <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.696	Zr $\sigma$ S	10.218	Mn <sub>2</sub> Rb <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.70	NiSbS	10.229	Mn <sub>2</sub> Tl <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.71	NiAsS	10.280	Cd <sub>2</sub> K <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.881	NiSbS	10.350	Cd <sub>2</sub> (NH <sub>4</sub> ) <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
5.9	NiSbS	10.382	Cd <sub>2</sub> Rb <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
6.358	H <sub>2</sub> $\sigma$	10.385	Cd <sub>2</sub> Tl <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
6.583	NaCl $\sigma$ <sub>3</sub>	10.533	(NH <sub>4</sub> ) <sub>2</sub> Mn <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
6.72	NaBr $\sigma$ <sub>3</sub>	10.536	(NH <sub>4</sub> ) <sub>2</sub> Ca <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
6.834	RbCN	10.57	Ca <sub>2</sub> Tl <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
6.916	AlAu <sub>4</sub>	10.570	Ca <sub>2</sub> Rb <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
7.17	Si $\sigma$ <sub>2</sub>	10.724	Ca <sub>2</sub> Cs <sub>2</sub> (S $\sigma$ <sub>4</sub> ) <sub>3</sub>
7.38	NaAlSi $\sigma$ <sub>4</sub>	11.859	Na <sub>3</sub> SbS <sub>4</sub> $\bullet$ 9H <sub>2</sub> $\sigma$
7.50	CaNa <sub>2</sub> Si $\sigma$ <sub>4</sub>	11.98	Na <sub>3</sub> SbS <sub>4</sub> $\bullet$ 9H <sub>2</sub> $\sigma$
7.705	KAl $\sigma$ <sub>2</sub>	12.04	Na <sub>3</sub> SbS <sub>4</sub> $\bullet$ 9H <sub>2</sub> $\sigma$
7.929	Ag <sub>3</sub> SN $\sigma$ <sub>3</sub>	12.368	InCl
8.14	BiCl <sub>3</sub>	12.992	HgSbBr
Organic			
5.64	C $\sigma$	11.64	NH <sub>4</sub> U $\sigma$ <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> C $\sigma$ $\sigma$ ) <sub>3</sub>
6.834	RbCN	13.28	NH <sub>4</sub> U $\sigma$ <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> N <sub>2</sub> $\sigma$ <sub>2</sub> ) <sub>3</sub>
10.653	NaAm $\sigma$ <sub>2</sub> (CH <sub>3</sub> C $\sigma$ $\sigma$ ) <sub>3</sub>	13.341	NH <sub>4</sub> U $\sigma$ <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> N <sub>2</sub> $\sigma$ <sub>2</sub> ) <sub>3</sub>
10.664	NaPu $\sigma$ <sub>2</sub> (CH <sub>3</sub> C $\sigma$ $\sigma$ ) <sub>3</sub>	13.54	[N(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> CH <sub>3</sub> ] <sub>2</sub> SnCl <sub>6</sub>
10.681	NaNp $\sigma$ <sub>2</sub> (CH <sub>3</sub> C $\sigma$ $\sigma$ ) <sub>3</sub>	15.53	[(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> CH <sub>3</sub> As] <sub>2</sub> CoCl <sub>4</sub>
10.688	NaU $\sigma$ <sub>2</sub> ( $\sigma$ <sub>2</sub> CCH <sub>3</sub> ) <sub>3</sub>	15.55	[(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> CH <sub>3</sub> As] <sub>2</sub> ZnCl <sub>4</sub>
10.692	NaU $\sigma$ <sub>2</sub> (CH <sub>3</sub> C $\sigma$ $\sigma$ ) <sub>3</sub>	15.557	[(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> CH <sub>3</sub> As] <sub>2</sub> NiCl <sub>4</sub>
10.77	N(CH <sub>2</sub> $\bullet$ CH <sub>2</sub> $\bullet$ NH <sub>3</sub> Cl) <sub>3</sub>	15.63	[(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> CH <sub>3</sub> As] <sub>2</sub> MnCl <sub>4</sub>
11.52	KU $\sigma$ <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> C $\sigma$ $\sigma$ ) <sub>3</sub>	15.65	[(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> CH <sub>3</sub> As] <sub>2</sub> FeCl <sub>4</sub>
11.60	[(CH <sub>3</sub> ) <sub>4</sub> N]SbCl <sub>6</sub>		

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 2 3 I<sub>2,3</sub> T<sup>5</sup> No. 199 Inorganic - 9  
 Organic - 0  
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Inorganic  
 6.3557 CoU 9.54 Hg<sub>3</sub>Te<sub>2</sub>Br<sub>2</sub>  
 8.937 Hg<sub>3</sub>S<sub>2</sub>Cl<sub>2</sub> 10.96 TiTe<sub>3</sub>θ<sub>8</sub>  
 9.06 Hg<sub>3</sub>Se<sub>2</sub>Cl<sub>2</sub> 11.17 SnTe<sub>3</sub>θ<sub>8</sub>  
 9.33 Hg<sub>3</sub>Te<sub>2</sub>Cl<sub>2</sub> 11.32 ZrTe<sub>3</sub>θ<sub>8</sub>  
 9.37 (Mn,Fe)<sub>2</sub>θ<sub>3</sub>

Organic  
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 $\frac{2}{m} \bar{3}$  Pm3 T<sub>h</sub><sup>1</sup> No. 200 Inorganic - 3  
 Organic - 0  
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Inorganic  
 8.311 Al<sub>5</sub>Cu<sub>6</sub>Mg<sub>2</sub> 9.605 Cd<sub>11</sub>Na<sub>2</sub>  
 8.552 Mg<sub>2</sub>Zn<sub>11</sub>

Organic  
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 $\frac{2}{m} \bar{3}$  Pn3 T<sub>h</sub><sup>2</sup> No. 201 Inorganic - 26  
 Organic - 0  
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Inorganic  
 6.32 PH<sub>3</sub> 10.60 (NH<sub>4</sub>)<sub>5</sub>Ce[Ni(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub>  
 6.41 AsH<sub>3</sub> 10.61 CeTl<sub>5</sub>[Co(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub>  
 9.56 Tl<sub>2</sub>Sb<sub>3</sub>θ<sub>9</sub> 10.62 Tl<sub>5</sub>Y[Co(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub>  
 9.58 KSbθ<sub>3</sub> 10.66 K<sub>5</sub>Ce[Cu(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub>  
 9.770 Bi<sub>6</sub>θ<sub>13</sub>•xH<sub>2</sub>θ 10.66 Rb<sub>5</sub>Ce[Co(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub>  
 10.03 KBiθ<sub>3</sub> 10.70 CeRb<sub>5</sub>[Cu(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub>  
 10.36 K<sub>5</sub>Y[Co(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub> 10.72 Tl<sub>5</sub>Y[Cu(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub>  
 10.38 K<sub>5</sub>Y[Ni(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub> 10.76 CeRb<sub>5</sub>[Ni(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub>  
 10.51 CeK<sub>5</sub>[Co(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub> 10.81 CeTl<sub>5</sub>[Cu(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub>  
 10.56 (NH<sub>4</sub>)<sub>5</sub>Ce[Co(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub> 10.85 CeCe<sub>5</sub>[Ni(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub>  
 10.57 CeTl<sub>5</sub>[Ni(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub> 10.94 CeCe<sub>5</sub>[Co(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub>  
 10.58 CeK<sub>5</sub>[Ni(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub> 11.02 CeCe<sub>5</sub>[Cu(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub>  
 10.59 CeTl<sub>5</sub>[Fe(NO<sub>2</sub>)<sub>6</sub>]<sub>2</sub> 16.01 [Ca<sub>5</sub>Fe<sub>6</sub>Tl<sub>2</sub>(Asθ<sub>4</sub>)<sub>12</sub>•4H<sub>2</sub>θ]

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 $\frac{2}{m} \bar{3}$  Fm3 T<sub>h</sub><sup>3</sup> No. 202 Inorganic - 28  
 Organic - 0  
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Inorganic  
 10.28 K<sub>2</sub>AgCo(NO<sub>2</sub>)<sub>6</sub> 10.75 Rb<sub>3</sub>Co(NO<sub>2</sub>)<sub>6</sub>  
 10.35 (NH<sub>4</sub>)<sub>2</sub>AgCo(NO<sub>2</sub>)<sub>6</sub> 10.75 Tl<sub>3</sub>Ir(NO<sub>2</sub>)<sub>6</sub>  
 10.36 CaK<sub>2</sub>Ni(NO<sub>2</sub>)<sub>6</sub> 10.774 (NH<sub>4</sub>)<sub>3</sub>Co(NO<sub>2</sub>)<sub>6</sub>  
 10.41 AgTl<sub>2</sub>Co(NO<sub>2</sub>)<sub>6</sub> 10.79 Rb<sub>3</sub>Ir(NO<sub>2</sub>)<sub>6</sub>  
 10.42 K<sub>2</sub>PbCo(NO<sub>2</sub>)<sub>6</sub> 10.85 Rb<sub>3</sub>Rh(NO<sub>2</sub>)<sub>6</sub>  
 10.43 Rb<sub>2</sub>AgCo(NO<sub>2</sub>)<sub>6</sub> 10.93 (NH<sub>4</sub>)<sub>3</sub>Rh(NO<sub>2</sub>)<sub>6</sub>  
 10.48 K<sub>3</sub>Co(NO<sub>2</sub>)<sub>6</sub> 10.93 Tl<sub>3</sub>Rh(NO<sub>2</sub>)<sub>6</sub>  
 10.59 K<sub>3</sub>Ir(NO<sub>2</sub>)<sub>6</sub> 11.06 Cs<sub>2</sub>NaY(NO<sub>2</sub>)<sub>6</sub>  
 10.61 K<sub>2</sub>B<sub>12</sub>H<sub>12</sub> 11.17 Cs<sub>3</sub>Co(NO<sub>2</sub>)<sub>6</sub>  
 10.65 K<sub>3</sub>Rh(NO<sub>2</sub>)<sub>6</sub> 11.18 Cs<sub>2</sub>NaPr(NO<sub>2</sub>)<sub>6</sub>  
 10.66 K<sub>2</sub>BaCo(NO<sub>2</sub>)<sub>6</sub> 11.19 Cs<sub>3</sub>Ir(NO<sub>2</sub>)<sub>6</sub>  
 10.67 K<sub>2</sub>PbCu(NO<sub>2</sub>)<sub>6</sub> 11.20 Cs<sub>2</sub>NaCe(NO<sub>2</sub>)<sub>6</sub>  
 10.744 Tl<sub>3</sub>Co(NO<sub>2</sub>)<sub>6</sub> 11.24 Cs<sub>2</sub>NaLa(NO<sub>2</sub>)<sub>6</sub>  
 10.75 (NH<sub>4</sub>)<sub>3</sub>Ir(NO<sub>2</sub>)<sub>6</sub> 11.32 Cs<sub>3</sub>Rh(NO<sub>2</sub>)<sub>6</sub>

Organic  
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$\frac{2}{m}\bar{3}$	Fd3 $T_h^4$	No. 203	Inorganic - 5 Organic - 2
Inorganic			
13.90	$Na_6Mg_2S_4(C_6O_3)_4$	17.86	$K_3TlF_6$
16.75	$Ca_4AlSi(S_6)_4F_{12}(OH) \cdot 12H_2O$	21.80	$(Co(NH_3)_6)_4Cu_5Cl_{17}$
17.71	$K_3InF_6$		
Organic			
13.90	$Na_6Mg_2S_4(C_6O_3)_4$	15.74	$Be_4C(CH_3COO)_6$

$\frac{2}{m}\bar{3}$	Im3 $T_h^5$	No. 204	Inorganic - 25 Organic - 0
Inorganic			
7.47	$Ga(OH)_3$	8.287	$As_2Co$
7.507	$Al_{12}(Cr, Mn)$	8.311	$As_3(Ni, Co, Fe, Cu)$
7.5255	$Al_{12}Tc$	8.4691	$As_3Ir$
7.5270	$Al_{12}Re$	9.034	$CoSb_3$
7.573	$Al_{12}Mo$	9.230	$RhSb_3$
7.5803	$Al_{12}W$	9.249	$IrSb_3$
7.5815	$Al_{12}Mo$	9.790	$Bi_4O_9 \cdot nH_2O$
7.706	$CoP_3$	11.337	$Be_{17}Ru_3$
7.819	$NiF_3$	11.342	$Be_{17}Os_3$
7.828	$N_2O_4$	13.914	$Al_5CuLi_3$
7.898	$Sc(OH)_3$	13.930	$Al_{0.7}LiZn_{1.3}$
7.939	$In(OH)_3$	14.16	$(Al, Zn)_{49}Mg_{32}$
8.206	$As_3(Co, Fe, Ni)$		
Organic			
.....			

$\frac{2}{m}\bar{3}$	Pa3 $T_h^6$	No. 205	Inorganic - 146 Organic - 21
Inorganic			
4.839	$MgO_2$	5.9665	$As_2Pt$
4.871	$ZnO_2$	5.969	$As_2Pt$
5.273	$Cd(O_2, OH)$	5.98	$As_2Pd$
5.313	$CdO_2$	5.982	$As_2Pd$
5.415	$FeS_2$	5.991	$(Ni, Cu)Se_2$
5.4172	$FeS_2$	6.002	$RhSe_2$
5.430	$(Fe, Ni)S_2$	6.034	$NiSe_2$
5.46	$NaO_2$	6.107	$MnS_2$
5.50	$Fe_{0.65}Ni_{0.35}S_2$	6.377	$RuTe_2$
5.53462	$CoS_2$	6.3985	$OsTe_2$
5.58	$(Ni, Fe, Co)S_2$	6.411	$IrTe_{2+x}$
5.585	$RhS_2$	6.414	$Ir_3Te_8$
5.59	$(Co, Fe)AsS$	6.430	$MnSe_2$
5.60	$(Co, Ni, Fe)AsS$	6.4400	$PtSb_2$
5.60	$RuS_2$	6.441	$RhTe_2$
5.6188	$OsS_2$	6.4584	$PdSb_2$
5.64	$CO_2$	6.6583	$AuSb_2$
5.644	$N_2$	6.68	$Bi_2Pd$
5.65	$CoS_2$	6.7022	$Bi_2Pt$
5.65	$OsS_2$	6.957	$MnTe_2$
5.66	$NiAsS$	7.302	$Ni(NO_3)_2$
5.661	$N_2$	7.410	$Co(NO_3)_2$
5.682	$P_2Si$	7.477	$Mg(NO_3)_2$
5.692	$NiAsS$	7.48	$SiP_2O_7$
5.693	$(Cu, Ni)S_2$	7.520	$GeP_2O_7$
5.6956	$P_2Pt$	7.535	$Cd(NO_3)_2$
5.73	$N_2O$	7.56	$Cd(NO_3)_2$
5.75	$NiS_2$	7.62	$Ca(NO_3)_2$
5.809	$C_2Th$	7.710	$KPF_6$
5.857	$CoSe_2$	7.7798	$Sr(NO_3)_2$
5.8588	$CoSe_2$	7.82	$TiP_2O_7$
5.933	$RuSe_2$	7.86	$Pb(NO_3)_2$
5.941	$As_2Pt$	7.89	$N_2H_6Cl_2$
5.945	$OsSe_2$	7.90	$NH_4PF_6$
5.957	$NiSe_2$	7.91	$SnP_2O_7$
5.960	$NiSe_2$	7.94	$TlPF_6$

Pa3 T<sub>h</sub><sup>6</sup> No. 205 (continued)

## Inorganic (continued)

8.03	PbP <sub>2</sub> θ <sub>7</sub>	12.010	SiI <sub>4</sub>
8.109	K <sub>2</sub> NaAlF <sub>6</sub>	12.026	TiI <sub>4</sub>
8.11	K <sub>2</sub> NaAlF <sub>6</sub>	12.040	GeI <sub>4</sub>
8.119	Ba(Nθ <sub>3</sub> ) <sub>2</sub>	12.156	Cd <sub>4</sub> P <sub>2</sub> Cl <sub>3</sub>
8.20	HfP <sub>2</sub> θ <sub>7</sub>	12.158	AlK(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
8.20	NaSbF <sub>6</sub>	12.196	CrK(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
8.22	CsPF <sub>6</sub>	12.21	NaAl(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
8.22	ZrP <sub>2</sub> θ <sub>7</sub>	12.223	GaK(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
8.252	ZrP <sub>2</sub> θ <sub>7</sub>	12.232	AlTL(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
8.338	CeP <sub>2</sub> θ <sub>7</sub>	12.240	NH <sub>4</sub> Al(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
8.606	UP <sub>2</sub> θ <sub>7</sub>	12.245	AlRb(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
8.721	ThP <sub>2</sub> θ <sub>7</sub>	12.258	GaTL(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
8.74	RbNθ <sub>3</sub>	12.26	SnI <sub>4</sub>
8.76	ZrV <sub>2</sub> θ <sub>7</sub>	12.263	CrTL(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
9.02	ThAs <sub>2</sub> θ <sub>7</sub>	12.268	NH <sub>4</sub> Ga(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
9.0409	(NH <sub>4</sub> ) <sub>3</sub> GaF <sub>6</sub>	12.270	GaRb(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
10.30	Cu(Brθ <sub>3</sub> ) <sub>2</sub> •6H <sub>2</sub> θ	12.276	NH <sub>4</sub> Cr(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
10.330	Zn(Clθ <sub>3</sub> ) <sub>2</sub> •6H <sub>2</sub> θ	12.281	CrRb(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
10.34	ZrCl <sub>4</sub>	12.309	(NH <sub>3</sub> θH)Al(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
10.340	Zn(Brθ <sub>3</sub> ) <sub>2</sub> •6H <sub>2</sub> θ	12.318	NH <sub>4</sub> Fe(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
10.342	Co(Brθ <sub>3</sub> ) <sub>2</sub> •6H <sub>2</sub> θ	12.32	CsRb(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
10.355	Co(Clθ <sub>3</sub> ) <sub>2</sub> •6H <sub>2</sub> θ	12.332	Cd <sub>4</sub> P <sub>2</sub> Br <sub>3</sub>
10.415	Mg(Brθ <sub>3</sub> ) <sub>2</sub> •6H <sub>2</sub> θ	12.352	AlCs(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
10.45	PtCl <sub>4</sub>	12.376	AlK(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
10.760	Mg(Clθ <sub>3</sub> ) <sub>2</sub> •6H <sub>2</sub> θ	12.391	Cd <sub>4</sub> As <sub>2</sub> Cl <sub>3</sub>
10.95	ZrBr <sub>4</sub>	12.402	CsGa(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
10.98	Ni(NH <sub>3</sub> ) <sub>6</sub> (Nθ <sub>3</sub> ) <sub>2</sub>	12.403	CrCs(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
11.05	SPBr <sub>3</sub>	12.408	(H <sub>2</sub> NθNH <sub>3</sub> )Al(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
11.273	TiBr <sub>4</sub>	12.439	CsV(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
11.30	[Co(NH <sub>3</sub> ) <sub>4</sub> (H <sub>2</sub> θ) <sub>2</sub> ]TiCl <sub>6</sub>	12.57	Mg(H <sub>2</sub> θ) <sub>6</sub> TeI <sub>6</sub>
11.42	Co(NH <sub>3</sub> ) <sub>6</sub> TlCl <sub>6</sub>	12.611	Hg <sub>4</sub> As <sub>2</sub> Br <sub>3</sub>
11.52	Co(NH <sub>3</sub> ) <sub>6</sub> PbCl <sub>6</sub>	12.640	Cd <sub>4</sub> As <sub>2</sub> Br <sub>3</sub>
11.54	Co(NH <sub>3</sub> ) <sub>6</sub> BiCl <sub>6</sub>	12.736	Cd <sub>4</sub> P <sub>2</sub> I <sub>3</sub>
11.765	HfI <sub>4</sub>	13.009	Hg <sub>4</sub> As <sub>2</sub> I <sub>3</sub>
11.79	Co(NH <sub>3</sub> ) <sub>6</sub> TlBr <sub>6</sub>	13.020	Cd <sub>4</sub> As <sub>2</sub> I <sub>3</sub>
11.91	GeI <sub>4</sub>	13.436	Hg <sub>4</sub> Sb <sub>2</sub> I <sub>3</sub>
11.93	Mg(H <sub>2</sub> θ) <sub>6</sub> TeBr <sub>6</sub>	13.485	Cd <sub>4</sub> Sb <sub>2</sub> I <sub>3</sub>

## Organic

5.64	Cθ <sub>2</sub>	12.44	[(CH <sub>3</sub> ) <sub>3</sub> S] <sub>2</sub> SnCl <sub>6</sub>
5.809	ThC <sub>2</sub>	12.504	NH <sub>3</sub> CH <sub>3</sub> Al(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
9.667	(C <sub>6</sub> H <sub>6</sub> ) <sub>2</sub> Cr	12.541	NH <sub>3</sub> CH <sub>3</sub> Cr(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ
9.73	(C <sub>6</sub> H <sub>6</sub> ) <sub>2</sub> V	12.831	[(CH <sub>3</sub> ) <sub>2</sub> C <sub>2</sub> H <sub>5</sub> S] <sub>2</sub> SnCl <sub>6</sub>
10.09	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>	13.20	[N(CH <sub>3</sub> ) <sub>3</sub> C <sub>2</sub> H <sub>5</sub> ] <sub>2</sub> SnCl <sub>6</sub>
10.109	C <sub>14</sub> H <sub>20</sub>	13.5	[C(NH <sub>2</sub> ) <sub>3</sub> ] <sub>2</sub> Tn(CH <sub>3</sub> Cθ <sub>2</sub> ) <sub>6</sub>
10.51	C <sub>6</sub> H <sub>6</sub> Br <sub>6</sub>	14.56	C <sub>6</sub> H <sub>15</sub> N <sub>3</sub>
10.82	C <sub>6</sub> (CN) <sub>6</sub>	16.20	N <sub>6</sub> P <sub>6</sub> (N[CH <sub>3</sub> ] <sub>2</sub> ) <sub>12</sub>
10.84	Ni(Cθ) <sub>4</sub>	20.33	Co <sub>4</sub> C(θCθC(CH <sub>3</sub> ) <sub>3</sub> ) <sub>6</sub>
12.17	NH <sub>3</sub> CH <sub>3</sub> Al(Sθ <sub>4</sub> ) <sub>2</sub> •12H <sub>2</sub> θ	20.53	[(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> )P] <sub>3</sub> Re <sub>3</sub> Cl <sub>9</sub>
12.21	[(CH <sub>3</sub> ) <sub>3</sub> NH] <sub>2</sub> SnCl <sub>6</sub>		

Z<sub>m</sub><sup>3</sup>Ia3 T<sub>h</sub><sup>7</sup> No. 206Inorganic - 57  
Organic - 1

## Inorganic

6.64	Si	9.93	AgTaF <sub>6</sub>
8.150	Be <sub>3</sub> N <sub>2</sub>	9.97	Mg <sub>3</sub> N <sub>2</sub>
8.60	TlHF <sub>2</sub>	10.032	θ <sub>2</sub> PtF <sub>6</sub>
9.384	(Mn,Fe) <sub>2</sub> θ <sub>3</sub>	10.117	In <sub>2</sub> θ <sub>3</sub>
9.400	(Fe,Mn) <sub>2</sub> θ <sub>3</sub>	10.135	Zr <sub>2</sub> θN <sub>2</sub>
9.43	Mn <sub>2</sub> θ <sub>3</sub>	10.14	In <sub>2</sub> θ <sub>3</sub>
9.436	Li <sub>5</sub> N <sub>3</sub> Si	10.15	KSnF <sub>6</sub>
9.480	ALLi <sub>3</sub> N <sub>2</sub>	10.17	Be <sub>3</sub> P <sub>2</sub>
9.613	GaLi <sub>3</sub> N <sub>2</sub>	10.29	KNbF <sub>6</sub>
9.614	GeLi <sub>5</sub> N <sub>3</sub>	10.29	KTaF <sub>6</sub>
9.700	Li <sub>5</sub> N <sub>3</sub> Ti	10.39	Lu <sub>2</sub> θ <sub>3</sub>
9.763	N <sub>2</sub> Zn <sub>3</sub>	10.41	Yb <sub>2</sub> θ <sub>3</sub>
9.81	Sc <sub>2</sub> θ <sub>3</sub>	10.435	Yb <sub>2</sub> θ <sub>3</sub>
9.845	Sc <sub>2</sub> θ <sub>3</sub>	10.488	Tm <sub>2</sub> θ <sub>3</sub>
9.85	AgSbF <sub>6</sub>	10.52	Tl <sub>2</sub> θ <sub>3</sub>
9.855	Sc <sub>2</sub> θ <sub>3</sub>	10.550	Er <sub>2</sub> θ <sub>3</sub>
9.93	AgNbF <sub>6</sub>	10.59	Tl <sub>2</sub> θ <sub>3</sub>

Ia3  $T_h^7$  No. 206 (continued)

## Inorganic (continued)

10.604	$Y_2O_3$	10.532	$Sm_2O_3$
10.607	$Ho_2O_3$	10.59	$Pm_2O_3$
10.62	$Y_2O_3$	11.03	$Am_2O_3$
10.65	$Dy_2O_3$	11.078	$Nd_2O_3$
10.667	$Dy_2O_3$	11.138	$Pr_2O_3$
10.688	$N_3U_2$	11.172	$Ce_2O_3$
10.700	$N_3U_2$	11.4	$La_2O_3$
10.71	$Tb_2O_3$	11.42	$Ca_3N_2$
10.81	$Cd_3N_2$	12.03	$Mg_3P_2$
10.813	$Gd_2O_3$	12.35	$As_2Mg_3$
10.86	$Eu_2O_3$	13.730	$Al(NO_3)_3 \cdot 7H_2O$
10.87	$Sm_2O_3$		

## Organic

15.92  $NaH(CH_3COO)_2$ 

4 3 2

P432  $O^1$  No. 207Inorganic - 0  
Organic - 0

.....

4 3 2

P4<sub>2</sub>32  $O^2$  No. 208Inorganic - 8  
Organic - 0

## Inorganic

9.76	$Cu_8SiS_6$	10.91	$Ag_8GeSe_6$
9.90	$Cu_8GeS_6$	10.96	$Ag_8SnSe_6$
10.17	$Cu_8SiSe_6$	11.07	$Ag_8SnSe_6$
10.86	$Ag_8SiSe_6$	13.402	$SiO_2$

## Organic

.....

4 3 2

F432  $O^3$  No. 209Inorganic - 1  
Organic - 0

## Inorganic

5.3880  $CdF_2$ 

## Organic

.....

4 3 2

F4<sub>1</sub>32  $O^4$  No. 210Inorganic - 1  
Organic - 4

## Inorganic

15.9  $Fe(CN)_2$ 

## Organic

15.9	$Fe(CN)_2$	18.91	$(C_6H_5)_3CClO_4$
18.87	$(C_6H_5)_3CBF_4$	24.61	$[Rh(C_5H_8(NH_2)_2)_3]KClO_4 \cdot 3 \cdot 12H_2O$

4 3 2

I432  $O^5$  No. 211Inorganic - 3  
Organic - 0

## Inorganic

5.591	$Ga_4Mn$	7.15	$(NH_4)_2SrCl_4$
6.016	$Hg_4Ni$		

1432 0<sup>5</sup> No. 211 (continued)

Organic

.....

4 3 2 P<sub>4,32</sub> 0<sup>6</sup> No. 212 (includes P<sub>4,32</sub> No. 213) Inorganic - 23  
Organic - 4

Inorganic

6.224	Cu <sub>5</sub> Si	8.203	LiGa <sub>5</sub> Ge <sub>8</sub>
6.273	Cu <sub>13</sub> Ge <sub>4</sub> Ni <sub>3</sub>	8.204	CoLi <sub>2</sub> Ge <sub>3</sub> Ge <sub>8</sub>
6.302	Mn	8.213	Ge <sub>3</sub> Zn <sub>2</sub> Ge <sub>8</sub>
6.356	CoZn	8.324	Co <sub>3</sub> (VGe <sub>4</sub> ) <sub>2</sub>
6.374	(Cr,Fe)(Cr,W)	8.331	LiFe <sub>5</sub> Ge <sub>8</sub>
6.43	Fe <sub>2</sub> Re <sub>3</sub>	8.3340	Co <sub>0.87</sub> V
6.535	Si <sub>2</sub> Sr	8.372	Li <sub>2</sub> ZnTi <sub>3</sub> Ge <sub>8</sub>
6.540	Si <sub>2</sub> Sr	8.377	CoLi <sub>2</sub> Ti <sub>3</sub> Ge <sub>8</sub>
6.919	AlAu <sub>4</sub>	8.535	CdLi <sub>2</sub> Ti <sub>3</sub> Ge <sub>8</sub>
6.923	AlAu <sub>3</sub>	9.72	Ag <sub>3</sub> AuS <sub>2</sub>
6.934	Ag <sub>3</sub> Al	10.253	Zr <sub>2</sub> S <sub>3</sub>
8.190	Li <sub>2</sub> ZnGe <sub>3</sub> Ge <sub>8</sub>		

Organic

8.3340	VC <sub>0.87</sub>	12.843	(CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub> SbBr <sub>2</sub>
12.743	(CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub> SbCl <sub>2</sub>	16.62	MgC <sub>2</sub> C <sub>2</sub> H <sub>2</sub> •3NH <sub>3</sub>

4 3 2 P<sub>4,32</sub> 0<sup>7</sup> No. 213 (see No. 212)

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4 3 2 I<sub>4,32</sub> 0<sup>8</sup> No. 214 Inorganic - 5  
Organic - 0

Inorganic

9.95	Ag <sub>3</sub> AuSe <sub>2</sub>	12.86	MgWGe <sub>4</sub>
10.38	Ag <sub>3</sub> AuTe <sub>2</sub>	12.879	Ca <sub>3</sub> Be <sub>3</sub> Li <sub>2</sub> (SiGe <sub>4</sub> ) <sub>3</sub> F <sub>2</sub>
12.650	LiAlGe <sub>2</sub>		

Organic

.....

4 3 m P<sub>4,3m</sub> T<sub>d</sub><sup>1</sup> No. 215 Inorganic - 40  
Organic - 4

Inorganic

3.878	CFe <sub>4</sub>	8.086	(Mg,Fe) <sub>5</sub> (Al,Fe) <sub>18</sub> Ge <sub>32</sub>
4.010	ND <sub>4</sub> Br	8.320	3Li <sub>2</sub> WGe <sub>4</sub> •Li <sub>7</sub> (LiW <sub>4</sub> Ge <sub>16</sub> )•4H <sub>2</sub> O
4.264	CuF	8.7023	Al <sub>4</sub> Cu <sub>9</sub>
5.268	Cu <sub>3</sub> (As,V)S <sub>4</sub>	8.89	Na <sub>2</sub> Zn <sub>3</sub> Al <sub>6</sub> Si <sub>6</sub> Ge <sub>28</sub> S <sub>3</sub>
5.28	Cu <sub>3</sub> (As,Cu,Fe,V)S <sub>4</sub>	8.97	Ag <sub>4</sub> Na <sub>2</sub> SrAl <sub>6</sub> Si <sub>6</sub> Ge <sub>28</sub> S <sub>3</sub>
5.301	Cu <sub>3</sub> (Fe,Ge)S <sub>4</sub>	8.98	Na <sub>8</sub> Al <sub>6</sub> Si <sub>6</sub> Ge <sub>24</sub> S <sub>4</sub>
5.3912	Cu <sub>3</sub> VS <sub>4</sub>	8.99	Be <sub>3</sub> Na <sub>2</sub> Al <sub>6</sub> Si <sub>6</sub> Ge <sub>28</sub> S <sub>3</sub>
5.50	Cu <sub>3</sub> NbS <sub>4</sub>	8.99	Ag <sub>4</sub> CaNa <sub>2</sub> Al <sub>6</sub> Si <sub>6</sub> Ge <sub>28</sub> S <sub>3</sub>
5.52	Cu <sub>3</sub> TaS <sub>4</sub>	9.00	Tl <sub>6</sub> Al <sub>4</sub> Si <sub>6</sub> Ge <sub>24</sub> S <sub>3</sub>
5.57	Cu <sub>3</sub> VS <sub>4</sub>	9.05	Na <sub>8</sub> Al <sub>6</sub> Si <sub>6</sub> Ge <sub>24</sub> S <sub>4</sub>
5.65	Cu <sub>3</sub> NbSe <sub>4</sub>	9.06	Ca <sub>4</sub> Al <sub>6</sub> Si <sub>6</sub> Ge <sub>28</sub> S <sub>3</sub>
5.67	Cu <sub>3</sub> TaSe <sub>4</sub>	9.06	Mn <sub>2</sub> Na <sub>2</sub> Al <sub>4</sub> Si <sub>6</sub> Ge <sub>24</sub> S <sub>3</sub>
5.865	BiF <sub>3</sub>	9.16	Na <sub>2</sub> Pb <sub>3</sub> Al <sub>4</sub> Si <sub>6</sub> Ge <sub>24</sub> S <sub>3</sub>
6.33	Cd(CN) <sub>2</sub>	10.102	Li <sub>10</sub> Pb <sub>3</sub>
7.317	CsAl <sub>4</sub> Be <sub>4</sub> B <sub>11</sub> (OH) <sub>4</sub> Ge <sub>25</sub>	10.64	K <sub>9</sub> H <sub>3</sub> (H <sub>2</sub> W <sub>12</sub> Ge <sub>40</sub> )•12H <sub>2</sub> O
7.68	Li <sub>3</sub> HGe <sub>7</sub> Ge <sub>16</sub> •4H <sub>2</sub> O	10.64	K <sub>8</sub> H <sub>4</sub> (H <sub>2</sub> W <sub>12</sub> Ge <sub>40</sub> )•12H <sub>2</sub> O
7.695	Tl <sub>3</sub> HGe <sub>7</sub> Ge <sub>16</sub> •4H <sub>2</sub> O	10.684	K <sub>8</sub> (H <sub>2</sub> W <sub>12</sub> Ge <sub>40</sub> )•9H <sub>2</sub> O
7.72	(NH <sub>4</sub> ) <sub>3</sub> HGe <sub>7</sub> Ge <sub>16</sub> •4H <sub>2</sub> O	10.684	K <sub>8</sub> (H <sub>2</sub> W <sub>12</sub> Ge <sub>40</sub> )•11H <sub>2</sub> O
7.74	Al <sub>4</sub> K(OH) <sub>4</sub> (AsGe <sub>4</sub> ) <sub>3</sub> •8H <sub>2</sub> O	11.14	Rb <sub>6</sub> H <sub>2</sub> (H <sub>2</sub> W <sub>12</sub> Ge <sub>40</sub> )•4H <sub>2</sub> O
7.93	Fe <sub>4</sub> K(OH) <sub>4</sub> (AsGe <sub>4</sub> ) <sub>3</sub> •6-8H <sub>2</sub> O	11.17	(NH <sub>4</sub> ) <sub>6</sub> H <sub>2</sub> (H <sub>2</sub> W <sub>12</sub> Ge <sub>40</sub> )•8H <sub>2</sub> O

P $\bar{4}$ 3m T $_d^1$  No. 215 (continued)

Organic			
3.878	Fe $_4$ C	8.811	P $_4$ O $_6$ [Ni(CO) $_3$ ] $_4$
6.33	Cd(CN) $_2$	12.22	Cu $_4$ Cl $_6$ [(C $_6$ H $_5$ ] $_3$ P $_3$ ) $_4$

$\bar{4}$  3 m

F $\bar{4}$ 3m T $_d^2$  No. 216

Inorganic - 151  
Organic - 2

Inorganic

3.615	BN	6.158	In $_2$ Te $_3$
4.357	CSi	6.36	(Ag,Cu)I
4.534	BP	6.37	HgTe
4.538	BP	6.396	Ag $_2$ HgI $_4$
4.55	BP	6.460	HgTe
4.777	AsB	6.465	InSb
4.8624	BeS	6.4760	InSb
4.867	BeS	6.478	CdTe
4.887	LiNZn	6.47877	InSb
5.139	BeSe	6.480	CdTe
5.181	Ge $_2$ S $_3$	6.486	AgI
5.217	Ni $_4$ -xS $_2$	6.71	Ni $_5$ Zr
5.241	PSi	6.93	AgCl $_4$
5.315	(Cu,Fe,Mo,Sn,Zn) $_4$ (S,As,Te,Sb) $_3$ - $_4$	7.01	AgCl $_4$
5.404	SrAs $_2$ S $_4$	7.059	Cu $_4$ InMg
5.416	CuCl	7.09	NaCl $_4$
5.416	(Zn,Fe)S	7.26	NaCl $_4$
5.426	Zn $_{0.73}$ Fe $_{0.27}$ S	7.273	Na $_8$ Al $_4$ Si $_4$ O $_{18}$
5.429	Ge $_2$ Se $_3$	7.388	CeMg $_3$
5.429	(Zn,Fe)S	7.388	Mg $_3$ Pr
5.431	Zn $_{0.66}$ Fe $_{0.34}$ S	7.493	LaMg $_3$
5.436	Zn $_2$ GeS $_4$	7.52	KCl $_4$
5.447	GaP	7.63	TlCl $_4$
5.462	AlP	7.69	NH $_4$ Cl $_4$
5.467	AlP	7.72	RbCl $_4$
5.50	CuCl	7.72	TlCl $_4$
5.606	MnS	7.747	Au $_5$ Ca
5.611	MnS	7.94	Na $_3$ W $_3$ F $_3$
5.626	BeTe	8.00	CsCl $_4$
5.639	AlAs	8.16	Na $_3$ Mo $_3$ F $_3$
5.646	AsGa	8.243	GaLiCr $_4$ O $_8$
5.646	Zn $_2$ GeSe $_4$	8.411	LiInCr $_4$ O $_8$
5.656	Ag $_2$ Bi $_2$ S $_4$	8.44	(NH $_4$ ) $_2$ VF $_5$ (H $_2$ O)
5.672	ZnSe	8.447	GaLiRh $_4$ O $_8$
5.690	Cu $_2$ SnSe $_4$	8.5	BaSr $_2$ W $_6$
5.6909	CuBr	8.53	Ba $_2$ SrW $_6$
5.741	Cu $_{1.8}$ Se	8.55	K $_3$ Mo $_3$ F $_3$
5.793	(Hg,Zn)(S,Se)	8.605	InLiRh $_4$ O $_8$
5.818	CdS	8.67	K $_3$ W $_3$ F $_3$
5.83	CuBr	8.922	(NH $_4$ ) $_3$ AlF $_6$
5.83	MnSe	8.96	Rb $_3$ W $_3$ F $_3$
5.835	CdS	9.00	Rb $_3$ Mo $_3$ F $_3$
5.852	Cu $_2$ Se	9.028	(NH $_4$ ) $_3$ CrF $_6$
5.858	HgS	9.058	(NH $_4$ ) $_3$ VF $_6$
5.86875	InP	9.12	(NH $_4$ ) $_3$ FeF $_6$
5.8717	HgS	9.12	(NH $_4$ ) $_3$ Mo $_3$ F $_3$
5.873	InP	9.33	Ce $_3$ W $_3$ F $_3$
5.886	Ge $_2$ Te $_3$	9.40	Ce $_3$ Mo $_3$ F $_3$
5.918	Hg(S,Se)	9.524	Hg $_2$ N(Cl,S $_4$ ,Mo $_4$ ,C $_3$ ) $\cdot$ H $_2$ O
5.994	Be $_5$ Pd	9.540	Li $_5$ Ni $_2$
6.048	AsIn	9.58	Hg $_2$ N $_2$ O $_2$ H $_2$ O
6.05	CdSe	9.99	CeNiP $_4$ $\cdot$ 6H $_2$ O
6.058	AsIn	10.02	CoCsP $_4$ $\cdot$ 6H $_2$ O
6.059	CuI	10.04	CeFeP $_4$ $\cdot$ 6H $_2$ O
6.080	HgSe	10.10	CeNiAs $_4$ $\cdot$ 6H $_2$ O
6.084	HgSe	10.17	CeFeAs $_4$ $\cdot$ 6H $_2$ O
6.087	AsIn $_2$ Te	10.178	CeMgAs $_4$ $\cdot$ 6H $_2$ O
6.0954	GaSb	10.18	CoCsAs $_4$ $\cdot$ H $_2$ O
6.097	AuBe $_5$	10.25	CeMnAs $_4$ $\cdot$ 6H $_2$ O
6.101	ZnTe	10.271	Zn(NH $_3$ ) $_4$ (Cl $_4$ ) $_2$
6.105	GaSb	10.53	Co(NH $_3$ ) $_6$ S $_4$ Br
6.11	AlSb	10.54	Cd(NH $_3$ ) $_4$ (Re $_4$ ) $_2$
6.115	Cu $_2$ HgI $_4$	10.557	[Cr(NH $_3$ ) $_5$ H $_2$ O]BrS $_4$
6.138	AlSb	10.73	Co(NH $_3$ ) $_6$ S $_4$ I
6.15	CuI	10.75	[Co(NH $_3$ ) $_5$ H $_2$ O]Cl $_3$ S $_4$

F43m T<sub>d</sub><sup>2</sup> No. 216 (continued)

## Inorganic (continued)

10.82	[Co(NH <sub>3</sub> ) <sub>6</sub> ]Cl <sub>3</sub> Se <sub>4</sub>	11.49	[Cr(NH <sub>3</sub> ) <sub>5</sub> H <sub>2</sub> O](Cl <sub>4</sub> ) <sub>3</sub>
10.83	[Co(NH <sub>3</sub> ) <sub>5</sub> H <sub>2</sub> O]I <sub>3</sub>	11.568	Cr(NH <sub>3</sub> ) <sub>6</sub> (Cl <sub>4</sub> ) <sub>3</sub>
10.83	Co(NH <sub>3</sub> ) <sub>6</sub> (Se <sub>4</sub> )Cl <sub>4</sub>	11.694	Co(NH <sub>3</sub> ) <sub>6</sub> (PF <sub>6</sub> ) <sub>3</sub>
10.902	Co(NH <sub>3</sub> ) <sub>6</sub> I <sub>3</sub>	13.848	Al <sub>13</sub> Si <sub>5</sub> O <sub>20</sub> (OH,F) <sub>18</sub> Cl
10.91	[Co(NH <sub>3</sub> ) <sub>5</sub> H <sub>2</sub> O]Cl <sub>4</sub> Se <sub>4</sub>	13.91	Al <sub>13</sub> Si <sub>5</sub> O <sub>20</sub> (OH,F) <sub>18</sub> Cl
10.917	Al <sub>13</sub> Cr <sub>4</sub> Si <sub>4</sub>	14.023	Ca <sub>12</sub> Be <sub>17</sub> O <sub>29</sub>
10.97	[Co(NH <sub>3</sub> ) <sub>6</sub> ]Cl <sub>4</sub> Se <sub>4</sub>	14.034	Al <sub>13</sub> Si <sub>5</sub> O <sub>20</sub> (OH,F) <sub>18</sub> Cl
11.21	Co(NH <sub>3</sub> ) <sub>6</sub> (BF <sub>4</sub> ) <sub>3</sub>	17.9550	Cu <sub>4</sub> Sn
11.234	Co(NH <sub>3</sub> ) <sub>6</sub> (BF <sub>4</sub> ) <sub>3</sub>	18.01	Na[Al <sub>13</sub> O <sub>4</sub> (OH) <sub>24</sub> (H <sub>2</sub> O) <sub>12</sub> ](SeO <sub>4</sub> ) <sub>4</sub> ·xH <sub>2</sub> O
11.34	Co(NH <sub>3</sub> ) <sub>5</sub> H <sub>2</sub> O(Cl <sub>4</sub> ) <sub>3</sub>	19.75	Li <sub>4</sub> Sn
11.400	Co(NH <sub>3</sub> ) <sub>6</sub> (Cl <sub>4</sub> ) <sub>3</sub>		

## Organic

4.357	SiC	9.574	C <sub>9</sub> H <sub>16</sub>
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4 3 m

I43m T<sub>d</sub><sup>3</sup> No. 217Inorganic - 52  
Organic - 7

## Inorganic

5.42	SiF <sub>4</sub>	9.763	OsTa
7.48	Zn <sub>4</sub> O(BO <sub>2</sub> ) <sub>6</sub>	10.01	Ag <sub>5</sub> Cd <sub>8</sub>
7.51	Tl <sub>3</sub> VSe <sub>4</sub>	10.21	(Cu,Fe,Ag) <sub>12</sub> As <sub>4</sub> S <sub>13</sub>
7.65	Tl <sub>3</sub> NbS <sub>4</sub>	10.221	Cu <sub>3</sub> AsS <sub>3</sub>
7.67	Tl <sub>3</sub> TaSe <sub>4</sub>	10.232	Cu <sub>12</sub> As <sub>4</sub> S <sub>13</sub>
7.74	Tl <sub>3</sub> VSe <sub>4</sub>	10.32	Cu <sub>3</sub> (Sb,As) <sub>3</sub> S <sub>3</sub>
7.85	Tl <sub>3</sub> NbSe <sub>4</sub>	10.346	Cu <sub>12</sub> Sb <sub>4</sub> S <sub>13</sub>
7.88	Tl <sub>3</sub> TaSe <sub>4</sub>	10.38	PbAs <sub>4</sub> Bi <sub>4</sub> S <sub>9</sub>
8.4716	U <sub>2</sub> F <sub>9</sub>	10.3908	Cu <sub>12</sub> Sb <sub>4</sub> S <sub>13</sub>
8.723	NaTh <sub>2</sub> F <sub>9</sub>	10.56	Al <sub>12</sub> Mg <sub>17</sub>
8.735	Cr	10.6	PbAs <sub>2</sub> S <sub>4</sub>
8.837	(Fe,Cr,Tl,Ni)	10.605	CuFeS <sub>2</sub>
8.86	Cu <sub>5</sub> Zn <sub>8</sub>	11.185	Lu <sub>5</sub> Mg <sub>24</sub>
8.912	Mn	11.208	Mg <sub>24</sub> Tm <sub>5</sub>
8.917	Na <sub>4</sub> Al <sub>3</sub> Si <sub>3</sub> O <sub>12</sub> Cl	11.224	Er <sub>5</sub> Mg <sub>24</sub>
9.55	MoRe <sub>4</sub>	11.233	Ho <sub>5</sub> Mg <sub>24</sub>
9.55	MoRe <sub>9</sub>	11.246	Dy <sub>5</sub> Mg <sub>24</sub>
9.58	Al <sub>5</sub> Re <sub>24</sub>	11.257	Mg <sub>24</sub> Y <sub>5</sub>
9.588	Re <sub>7</sub> W <sub>3</sub>	11.283	Mg <sub>24</sub> Tb <sub>5</sub>
9.588	Re <sub>3</sub> W	11.72	Cs <sub>3</sub> H <sub>2</sub> (V <sub>2</sub> Mo <sub>10</sub> P <sub>6</sub> O <sub>40</sub> )·0-2H <sub>2</sub> O
9.670	Nb <sub>4</sub> Re <sub>6</sub>	11.72	Cs <sub>3</sub> H(SiMo <sub>6</sub> W <sub>6</sub> O <sub>40</sub> )·0-2H <sub>2</sub> O
9.670	Nb <sub>3</sub> Re <sub>7</sub>	11.78	Cs <sub>3</sub> H(SiW <sub>12</sub> O <sub>40</sub> )·0-2H <sub>2</sub> O
9.700	Os <sub>0.6</sub> Ta <sub>0.4</sub>	11.81	Cs <sub>3</sub> H(PMo <sub>6</sub> W <sub>6</sub> O <sub>40</sub> )·0-2H <sub>2</sub> O
9.711	Re <sub>7</sub> Ta <sub>3</sub>	11.81	Cs <sub>3</sub> (Mo <sub>6</sub> W <sub>6</sub> P <sub>6</sub> O <sub>40</sub> )·0-2H <sub>2</sub> O
9.711	Re <sub>3</sub> Ta	12.13	H <sub>3</sub> (Mo <sub>6</sub> W <sub>6</sub> P <sub>6</sub> O <sub>40</sub> )·5H <sub>2</sub> O
9.713	Hf <sub>5</sub> Re <sub>24</sub>	15.90	MgNa <sub>21</sub> (SO <sub>4</sub> ) <sub>10</sub> Cl <sub>3</sub>

## Organic

7.021	(CH <sub>2</sub> ) <sub>6</sub> N <sub>4</sub>	10.57	(CH <sub>3</sub> ) <sub>3</sub> PtCl
7.09	C(N <sub>2</sub> ) <sub>4</sub>	13.08	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> P·CuI
10.14	[(CH <sub>3</sub> ) <sub>3</sub> P+OH] <sub>4</sub>	13.11	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> As·CuI
10.165	(CH <sub>3</sub> ) <sub>3</sub> P+OH		

4 3 m

P43n T<sub>d</sub><sup>4</sup> No. 218Inorganic - 11  
Organic - 0

## Inorganic

6.005	Ag <sub>3</sub> P <sub>6</sub>	8.888	Na <sub>4</sub> Al <sub>3</sub> Si <sub>3</sub> O <sub>12</sub> Cl
6.131	Ag <sub>3</sub> As <sub>6</sub>	9.06	Na <sub>8-x</sub> Al <sub>6</sub> Si <sub>6</sub> O <sub>24</sub> S <sub>2-4</sub>
8.131	Zn <sub>4</sub> Be <sub>3</sub> Si <sub>3</sub> O <sub>12</sub> S	9.12	Na <sub>6</sub> (Ca,K) <sub>2</sub> (Al <sub>6</sub> Si <sub>6</sub> O <sub>24</sub> )(SO <sub>4</sub> ,Cl) <sub>2</sub>
8.27	(Mn,Fe,Zn) <sub>4</sub> (BeSi <sub>6</sub> ) <sub>3</sub> S	9.571	Li <sub>7</sub> MnN <sub>4</sub>
8.68	(Li,Na) <sub>8-x</sub> Al <sub>6</sub> Si <sub>6</sub> O <sub>24</sub> S <sub>2-4</sub>	9.604	Li <sub>7</sub> N <sub>4</sub> V
8.886	HB <sub>2</sub>		

## Organic

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$\bar{4} 3 m$		$F\bar{4}3c$	$T_d^5$	No. 219	Inorganic - 23
					Organic - 0
Inorganic					
11.935	$Cu_3B_7\theta_{13}Cl$			12.120	$Co_3B_7\theta_{13}Cl$
11.955	$Cu_3B_7\theta_{13}Br$			12.121	$Cr_3B_7\theta_{13}Cl$
12.019	$Ni_3B_7\theta_{13}Cl$			12.153	$Cr_3B_7\theta_{13}Br$
12.035	$Ni_3B_7\theta_{13}Br$			12.171	$Cr_3B_7\theta_{13}I$
12.046	$Ni_3B_7\theta_{13}I$			12.190	$Fe_3B_7\theta_{13}Br$
12.065	$Zn_3B_7\theta_{13}Cl$			12.225	$Fe_3B_7\theta_{13}I$
12.079	$Mg_3B_7\theta_{13}Br$			12.301	$Mn_3B_7\theta_{13}Br$
12.091	$Zn_3B_7\theta_{13}I$			12.32	$Mn_3B_7\theta_{13}I$
12.1	$Mg_3B_7\theta_{13}Cl$			12.501	$Cd_3B_7\theta_{13}Br$
12.104	$Zn_3B_7\theta_{13}Br$			12.56	$Cd_3B_7\theta_{13}I$
12.108	$Co_3B_7\theta_{13}Br$			26.46	$Ba(Cl\theta_2)_2 \cdot 5Ba(NO_3)_2 \cdot 12H_2O$
12.119	$Co_3B_7\theta_{13}I$				

Organic

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$\bar{4} 3 m$		$I\bar{4}3d$	$T_d^6$	No. 220	Inorganic - 82
					Organic - 4
Inorganic					
8.0885	$C_3U_2$			9.150	$BaPr_2Se_4$
8.129	$C_3Pu_2$			9.186	$BaCe_2Se_4$
8.197	$P_4U_3$			9.258	$BaLa_2Se_4$
8.445	$Am_2S_3$			9.32	$Rb_4\theta_6$
8.4543	$Pu_2S_3$			9.350	$Bi_4U_3$
8.455	$Ce_2C_3$			9.372	$Sb_4Th_3$
8.507	$As_4U_3$			9.397	$U_3Te_4$
8.514	$As_4U_3$			9.611	$AsCu_3$
8.524	$Nd_3S_4$			9.619	$La_2Te_3$
8.537	$Eu_3S_4$			9.628	$La_3Te_4$
8.556	$Sm_3S_4$			9.713	$Cu_{15}Si_4$
8.594	$Pr_3S_4$			9.88	$Ce_4\theta_6$
8.617	$P_4Th_3$			10.258	$MnPb_3(P\theta_4)_2(S\theta_4)$
8.6250	$Ce_3S_4$			10.296	$CaPb_3(P\theta_4)_2(S\theta_4)$
8.6347	$Ce_2S_3$			10.299	$MgPb_3(P\theta_4)_2(S\theta_4)$
8.718	$Gd_3Se_4$			10.300	$Bi_4Si_3\theta_{12}$
8.724	$La_2S_3$			10.315	$CdPb_3(P\theta_4)_2S\theta_4$
8.730	$La_3S_4$			10.356	$CoPb_3(P\theta_4)_2(S\theta_4)$
8.785	$Sm_2Se_3$			10.364	$BiPb_3(P\theta_4)_3$
8.785	$AgSm_2Se_{3.5}$			10.369	$Pb_3Sr(P\theta_4)_2(S\theta_4)$
8.817	$C_3La_2$			10.422	$CuPb_3(P\theta_4)_2(S\theta_4)$
8.843	$As_4Th_3$			10.434	$NiPb_3(P\theta_4)_2(S\theta_4)$
8.854	$AgNd_2Se_{3.5}$			10.443	$Pb_4(P\theta_4)_2(S\theta_4)$
8.859	$Nd_3Se_4$			10.449	$Pb_3Zn(P\theta_4)_2(S\theta_4)$
8.895	$SrGd_2Se_4$			10.470	$BiPb_3(As\theta_4)(P\theta_4)_2$
8.902	$AgPr_2Se_{3.5}$			10.479	$BiPb_3(V\theta_4)(P\theta_4)_2$
8.927	$Pr_3Se_4$			10.514	$Pb_4(P\theta_4)_2(Cr\theta_4)$
8.931	$SrSm_2Se_4$			10.527	$Bi_4(Ge\theta_4)_3$
8.954	$AgCe_2Se_{3.5}$			10.578	$BiPb_3(As\theta_4)_2P\theta_4$
8.973	$Ce_3Se_4$			10.609	$BiPb_3(V\theta_4)_2P\theta_4$
8.989	$SrNd_2Se_4$			10.668	$BiPb_3(As\theta_4)_3$
8.99	$Ac_2S_3$			10.692	$BiPb_3(V\theta_4)(As\theta_4)_2$
9.019	$SrPr_2Se_4$			10.715	$BiPb_3(V\theta_4)_2As\theta_4$
9.026	$AgLa_2Se_{3.5}$			10.733	$BiPb_3(V\theta_4)_3$
9.055	$La_3Se_4$			10.781	$Ge_4Li_{15}$
9.060	$SrCe_2Se_4$			11.97	$Ca_{12}Al_{14}\theta_{33}$
9.095	$Sb_4U_3$			12.02	$Ca_{12}Al_{14}\theta_{33}$
9.11	$Th_4H_{15}$			13.32	$Na_{15}Pb_4$
9.112	$Sb_4U_3$			13.66	$Al_4(P_4\theta_{12})_3$
9.120	$BaNd_3Se_4$			13.729	$Al(P\theta_3)_3$
9.124	$SrLa_2Se_4$			21.73	$U_4\theta_9$

Organic

8.0885	$U_2C_3$	8.817	$La_2C_3$
8.129	$Pu_2C_3$	13.78	$(NO_2)_3C \cdot CH_3$

$\frac{4}{m} \frac{3}{m} \frac{2}{m}$	Pm3m	$O_h^1$	No. 221	Inorganic - 573	Organic - 5
Inorganic					
2.611	BeCo		3.619	AgY	
2.71	BeCu		3.622	SmZn	
2.819	BePd		3.629	YbZn	
2.83	AlNi		3.632	HgTm	
2.833	Co(Mn <sub>0.5</sub> Si <sub>0.5</sub> )		3.640	CdLu	
2.87	CoGa		3.645	ErHg	
2.879	AlNi		3.647	Co <sub>3</sub> Ta	
2.879	GaNi		3.6476	AgGd	
2.88	AlRe		3.660	HgHo	
2.904	MnV		3.663	CdTm	
2.948	CuZn		3.667	NdZn	
2.95	AlRu		3.669	AgSm	
2.9630	RhSi		3.672	DyHg	
2.968	AlRh		3.677	CdEr	
2.986	LiPd		3.678	PrZn	
2.994	CuPd		3.68	YAlO <sub>3</sub>	
3.004	GaIr		3.682	HgY	
3.005	AlOs		3.6826	AlDy	
3.010	GaRu		3.684	AgSm	
3.03	AlRu		3.685	CdEr	
3.049	AlPd		3.690	HgTb	
3.06	KF		3.695	CdHo	
3.06	RuTi		3.70	DyMnO <sub>3</sub>	
3.07	OsTi		3.701	CdHo	
3.099	InNi		3.704	CeZn	
3.10	AlCu <sub>2</sub> Sc		3.707	CdY	
3.17	MgPd		3.711	CdDy	
3.171	NiSc		3.711	AgNd	
3.203	RuSc		3.711	TlTm	
3.206	IrSc		3.715	ErTl	
3.206	RhSc		3.716	CdDy	
3.222	AuMn		3.719	GdHg	
3.256	CuSc		3.72	AgNd	
3.270	PtSc		3.7208	AlGd	
3.28	AgMg		3.7218	Li <sub>x</sub> W <sub>3</sub>	
3.283	PdSc		3.722	CdY	
3.29	RbF		3.725	CdTb	
3.315	HgMn		3.731	HgYb	
3.318	HgMn		3.734	CdTb	
3.3233	Au <sub>1.05</sub> Cd <sub>0.95</sub>		3.735	HoTl	
3.33	AgCd		3.735	HgYb	
3.35	ScZn		3.735	AgPr	
3.370	AuSc		3.739	AlSm	
3.39	CsF		3.74	AlNd	
3.415	CuTm		3.74	KBr	
3.431	CuEr		3.742	ReO <sub>3</sub>	
3.447	CuHo		3.743	DyTl	
3.461	CuDy		3.744	MgTm	
3.479	CuTb		3.744	HgSm	
3.479	CuY		3.7478	AuCu <sub>3</sub>	
3.480	HgSc		3.748	CdGd	
3.491	LuZn		3.749	RbCl	
3.503	CuGd		3.75	InNi <sub>3</sub>	
3.51	CdSc		3.751	TlY	
3.51	Ni <sub>3</sub> Si		3.755	CdGd	
3.515	TmZn		3.755	H <sub>0.5</sub> W <sub>3</sub>	
3.529	LiPb		3.756	ErMg	
3.533	ErZn		3.758	AgCe	
3.546	HoZn		3.76	CdTlO <sub>3</sub>	
3.548	DyZn		3.76	CaVO <sub>3</sub>	
3.5522	FeNi		3.760	LaZn	
3.562	DyZn		3.760	TbTl	
3.566	GeNi <sub>3</sub>		3.770	CdSm	
3.567	(Co <sub>0.83</sub> Fe <sub>0.17</sub> ) <sub>3</sub> V		3.770	HoMg	
3.5673	AlNi <sub>3</sub>		3.772	HgNd	
3.576	TbZn		3.773	B <sub>0.5</sub> InNi <sub>3</sub>	
3.578	YZn		3.775	Cr <sub>3</sub> Pt	
3.58	KCl		3.777	NdCoO <sub>3</sub>	
3.59	MnNi <sub>3</sub>		3.7797	GdTl	
3.600	GdZn		3.780	CeAlO <sub>3</sub>	
3.607	HgLu		3.780	HgNd	
3.608	AgDy		3.784	DyMg	
3.61	KCl		3.7866	DyIn	
3.610	AlF <sub>3</sub> •H <sub>2</sub> O		3.789	MgY	



Pm3m  $O_h^1$  No. 221 (continued)

## Inorganic (continued)

3.79	CaV $\epsilon_3$	3.890	Pt $_3$ Ti
3.79	LaAl $\epsilon_3$	3.891	MnPt $_3$
3.791	HgPr	3.893	CeTl
3.795	Fe $_4$ N	3.893	Pt $_3$ Zn
3.796	LiEuH $_3$	3.896	Mo $\epsilon$ F $_2$
3.796	MgTb	3.896	Ta $\epsilon_2$ F
3.798	Ti $\epsilon$ F $_2$	3.897	(Ce,K)Ti $\epsilon_3$
3.799	HgPr	3.897	NaNb $\epsilon_3$
3.80	Mn $_4$ N	3.898	MgPr
3.80	NdMn $\epsilon_3$	3.898	GaMn $_3$ N
3.800	CdSm	3.8985	MoF $_3$
3.803	CaTi $\epsilon_3$	3.899	LaFe $\epsilon_3$
3.804	AgLa	3.90	CeV $\epsilon_3$
3.808	CeHg	3.90	LaFe $\epsilon_3$
3.808	InYb	3.90	LaGa $\epsilon_3$
3.8086	CdYb	3.90	NdV $\epsilon_3$
3.81	(Ca,Na)(Ti,Nb) $\epsilon_3$	3.90	PrV $\epsilon_3$
3.810	CdNd	3.900	Rh $_3$ Sc
3.812	EuZn	3.901	Nb $\epsilon_2$ F
3.813	SmTl	3.9012	TaF $_3$
3.815	Cu $_3$ N	3.902	Nb $\epsilon_2$ F
3.818	GdMg	3.902	SrTi $\epsilon_{2.5}$
3.82	GdMn $\epsilon_3$	3.903	NbF $_3$
3.82	PrMn $\epsilon_3$	3.903	(La,Rb)Ti $\epsilon_3$
3.826	CeHg	3.9049	SrTi $\epsilon_3$
3.826	TlYb	3.905	CdLa
3.828	TlYb	3.905	EuTi $\epsilon_3$
3.828	ThTe	3.906	CuMn $_3$ N
3.83	Mn $_3$ Pt	3.907	(La,K)Ti $\epsilon_3$
3.830	CdPr	3.908	CeFe $\epsilon_3$
3.830	GdIn	3.91	LaV $\epsilon_3$
3.831	CoPt $_3$	3.91	RbCl
3.833	LiSrH $_3$	3.916	Pt $_3$ Ti
3.837	HgLa	3.92	LaTi $\epsilon_3$
3.838	TlCl	3.922	LaTl
3.838	Tl $_7$ Sb $_7\epsilon_6$ (OH) $_{30}$	3.9249	CMn $_3$ Zn
3.845	MgSm	3.93	CaSn $\epsilon_3$
3.848	FePd $_3$	3.93	SrRu $\epsilon_3$
3.848	NdTl	3.930	HgSr
3.848	SrV $\epsilon_{2.5}$	3.9322	TiZn $_3$
3.851	NdGa $\epsilon_3$	3.934	NbZn $_3$
3.853	CaTi $\epsilon_3$	3.936	LaTl
3.86	AlCe	3.94	LaRh $\epsilon_3$
3.86	SbTl	3.94	KI
3.862	(Ca,Ce,Na)(Nb,Ti) $\epsilon_3$	3.958	Pt $_3$ Sc
3.8622	NaW $\epsilon_3$	3.960	CdEu
3.863	PrGa $\epsilon_3$	3.965	Sr $_2$ NbV $\epsilon_6$
3.864	HgLa	3.9675	Sr $_2$ TaV $\epsilon_6$
3.865	CdCe	3.970	EuTl
3.867	PrFe $\epsilon_3$	3.970	LaMg
3.869	AlCMn $_3$	3.973	KMgF $_3$
3.869	(La,Li)Ti $\epsilon_3$	3.975	EuTl
3.869	PrTl	3.98	BaTi $\epsilon_3$
3.869	SrFe $\epsilon_3$	3.981	Sr $_{0.7}$ Nb $\epsilon_3$
3.87	Pt $_3$ V	3.981	Pd $_3$ Sc
3.87	Ta $\epsilon_{0.82}$	3.9846	TlBr
3.87	TiCl $_4 \cdot 4NH_3$	3.988	Ru $_3$ U
3.873	(La,Na)Ti $\epsilon_3$	3.9885	KTa $\epsilon_3$
3.874	CeCr $\epsilon_3$	3.99	BiTl
3.8755	Cr $_3$ GaN	3.991	Rh $_3$ U
3.8758	NH $_4$ Cl	3.993	Pt $_3$ Sn
3.876	AlPt $_3$	3.994	TlCN
3.879	CeGa $\epsilon_3$	3.996	LiBaF $_3$
3.88	LaMn $\epsilon_3$	4.00	CaZr $\epsilon_3$
3.880	CaTa $\epsilon_3$	4.00	CoPb $_2$ W $\epsilon_6$
3.880	EuHg	4.007	BaFe $\epsilon_3$
3.880	SnTa $\epsilon_3$	4.01	KMgF $_3$
3.881	MgNd	4.011	CdSr
3.882	(La,Ag)Ti $\epsilon_3$	4.011	KNiF $_3$
3.883	(La,Tl)Ti $\epsilon_3$	4.0118	BaTi $\epsilon_3$
3.888	La $_{0.7}$ Ti $\epsilon_3$	4.013	KNb $\epsilon_3$
3.89	LaCr $\epsilon_3$	4.016	KNiF $_3$
3.89	LaFe $\epsilon_3$	4.016	Sr $_{0.95}$ Nb $\epsilon_3$
3.89	SmV $\epsilon_3$	4.0195	AgMn $_3$ N

Pm3m  $O_h^1$  No. 221 (continued)

## Inorganic (continued)

4.023	Pb <sub>2</sub> MnNb <sub>6</sub>	4.137	B <sub>6</sub> Ce
4.023	Ir <sub>3</sub> U	4.138	TlCoF <sub>3</sub>
4.023	LiBaH <sub>3</sub>	4.138	B <sub>6</sub> Yb
4.025	Pb <sub>3</sub> NiNb <sub>2</sub> O <sub>9</sub>	4.1383	Pd <sub>3</sub> Pr
4.025	Pb(Pd,Au) <sub>3</sub>	4.139	Rh <sub>3</sub> Th
4.032	SrTl	4.14	B <sub>6</sub> Dy
4.033	SrSnO <sub>3</sub>	4.140	B <sub>6</sub> Yb
4.034	Si <sub>3</sub> U	4.1410	B <sub>6</sub> Ce
4.0358	LuPd <sub>3</sub>	4.1450	B <sub>6</sub> Ca
4.0398	Pd <sub>3</sub> Yb	4.146	UO <sub>3</sub>
4.041	Pb <sub>3</sub> MgNb <sub>2</sub> O <sub>9</sub>	4.1468	B <sub>6</sub> Yb
4.0505	Ba <sub>2</sub> NbVO <sub>6</sub>	4.147	BaHfO <sub>3</sub>
4.053	Ba <sub>2</sub> TaVO <sub>6</sub>	4.147	B <sub>6</sub> La
4.0542	ErPd <sub>3</sub>	4.15	B <sub>6</sub> Gd
4.058	KZnF <sub>3</sub>	4.150	B <sub>6</sub> Si
4.059	NH <sub>4</sub> Br	4.153	B <sub>6</sub> Ca
4.06	La(Zr <sub>0.5</sub> Mg <sub>0.5</sub> )O <sub>3</sub>	4.153	B <sub>6</sub> La
4.060	ND <sub>4</sub> Br	4.158	KCrF <sub>3</sub>
4.062	RbCoF <sub>3</sub>	4.16	B <sub>6</sub> Th
4.0620	HoPd <sub>3</sub>	4.165	Mo <sub>2</sub> N
4.063	CsNH <sub>2</sub>	4.1654	HgTi <sub>3</sub>
4.063	SrHfO <sub>3</sub>	4.174	RbFeF <sub>3</sub>
4.064	HoPd <sub>3</sub>	4.175	B <sub>6</sub> Eu
4.064	HoPt <sub>3</sub>	4.180	Ba(Y <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.0684	DyPd <sub>3</sub>	4.186	KMnF <sub>3</sub>
4.069	KCoF <sub>3</sub>	4.187	Ba(Lu <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.072	BaCoO <sub>2.23</sub>	4.187	B <sub>6</sub> Sr
4.072	DyPt <sub>3</sub>	4.1899	BaZrO <sub>3</sub>
4.072	Pb(Ta <sub>0.5</sub> Sc <sub>0.5</sub> )O <sub>3</sub>	4.190	KMnF <sub>3</sub>
4.074	Pd <sub>3</sub> Y	4.192	Ba(Yb <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.075	Pt <sub>3</sub> Y	4.198	Ge <sub>3</sub> U
4.077	SrHfO <sub>3</sub>	4.1984	B <sub>6</sub> Sr
4.0773	Pd <sub>3</sub> Tb	4.2	CaPb <sub>2</sub> WO <sub>6</sub>
4.09	RbBr	4.20	B <sub>6</sub> Sr
4.093	B <sub>6</sub> Y	4.201	Ba(Tm <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.0938	GdPd <sub>3</sub>	4.205	Ge <sub>3</sub> U
4.094	B <sub>6</sub> Tb	4.206	TlI
4.0952	EuPd <sub>3</sub>	4.208	Ba(Er <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.096	SrZrO <sub>3</sub>	4.21	CsHF <sub>2</sub>
4.0960	B <sub>6</sub> Ho	4.21	TlNO <sub>2</sub>
4.097	B <sub>6</sub> Gd	4.2101	NbO
4.0976	B <sub>6</sub> Dy	4.211	Nb <sub>3</sub> Si
4.1	Cd <sub>2</sub> PbWO <sub>6</sub>	4.215	Al <sub>3</sub> Er
4.10	CsCl	4.215	BaCd
4.101	SrZrO <sub>3</sub>	4.216	Ba(Ho <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.101	B <sub>6</sub> Th	4.224	Ba(Dy <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.102	SrZrO <sub>3</sub>	4.229	Ba(Tb <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.1053	Pd <sub>3</sub> Sm	4.2325	B <sub>6</sub> K
4.110	B <sub>6</sub> Er	4.235	LaPd <sub>3</sub>
4.110	B <sub>6</sub> Gd	4.239	NH <sub>4</sub> MnF <sub>3</sub>
4.110	Pd <sub>4</sub> Th	4.242	Ba(Gd <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.110	B <sub>6</sub> Th	4.243	Ba(Eu <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.1132	B <sub>6</sub> Y	4.243	RbMnF <sub>3</sub>
4.114	BaSnO <sub>3</sub>	4.248	Ba(Sm <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.116	B <sub>6</sub> Nd	4.249	Ga <sub>3</sub> U
4.1168	BaSnO <sub>3</sub>	4.252	B <sub>6</sub> Ba
4.12	B <sub>6</sub> Lu	4.262	Al <sub>3</sub> Np
4.120	KFeF <sub>3</sub>	4.262	Al <sub>3</sub> Pu
4.121	Ba(Sc <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>	4.265	BaPbO <sub>3</sub>
4.121	CsCl	4.2680	B <sub>6</sub> Ba
4.1220	N <sub>4</sub> W <sub>3</sub>	4.27	Al <sub>3</sub> U
4.123	B <sub>6</sub> Pr	4.277	Ba(Nd <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.124	La(Zr <sub>0.5</sub> Ca <sub>0.5</sub> )O <sub>3</sub>	4.28	BaTbO <sub>3</sub>
4.125	B <sub>6</sub> Sm	4.28	SrCeO <sub>3</sub>
4.126	B <sub>6</sub> Nd	4.280	(NH <sub>4</sub> ,Li)I
4.1264	NdPd <sub>3</sub>	4.285	Ba(Fr <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.1278	CePd <sub>3</sub>	4.285	BaTbO <sub>3</sub>
4.128	B <sub>6</sub> Ho	4.287	Al <sub>3</sub> U
4.129	(NH <sub>4</sub> )CoF <sub>3</sub>	4.29	B <sub>6</sub> Ba
4.129	B <sub>6</sub> Pr	4.29	CsCN
4.129	B <sub>6</sub> Sm	4.293	Ba(Ce <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>
4.130	B <sub>6</sub> Ce	4.296	CsBr
4.132	B <sub>6</sub> Pr	4.296	LiIO <sub>2</sub> O
4.133	BaHg	4.298	Ba(La <sub>0.5</sub> Nb <sub>0.5</sub> )O <sub>3</sub>

Pm3m  $O_h^1$  No. 221 (continued)

## Inorganic (continued)

4.299	KU $\theta_3$	4.732	In $_3$ La
4.302	KCdF $_3$	4.733	NdTl $_3$
4.311	CsSH	4.7345	In $_3$ La
4.34	CsN $\theta_2$	4.742	CaSn $_3$
4.34	RbI	4.7445	EuSn $_3$
4.346	SiU $_3$	4.747	PrTl $_3$
4.348	HgNH $_2$ Br	4.767	CeTl $_3$
4.35	BaAm $\theta_3$	4.7694	LaSn $_3$
4.363	BaPr $\theta_3$	4.782	LaSn $_3$
4.3652	Hg $_3$ Zr	4.787	Pb $_3$ U
4.372	AlZr $_3$	4.804	CaTl $_3$
4.373	BaPu $\theta_3$	4.806	LaTl $_3$
4.38	NH $_4$ I	4.806	Ag $_3$ SBr
4.384	BaNp $\theta_3$	4.81	CsPbF $_3$
4.386	BaCe $\theta_3$	4.823	Pb $_3$ Y
4.3874	BaU $\theta_3$	4.828	GdPb $_3$
4.40	NH $_4$ N $\theta_3$	4.835	SmPb $_3$
4.446	CsSeH	4.852	NdPb $_3$
4.452	RbCaF $_3$	4.853	Ca $_3$ Pb
4.47	KI $\theta_3$	4.855	Pb $_3$ Th
4.489	BaTh $\theta_3$	4.862	Pb $_3$ Yb
4.500	GaPu $_3$	4.867	Pb $_3$ Pr
4.52	NH $_4$ I $\theta_3$	4.874	CePb $_3$
4.523	CsCaF $_3$	4.901	CaPb $_3$
4.53	RbI $\theta_3$	4.903	LaPb $_3$
4.5526	In $_3$ Lu	4.903	Ag $_3$ SI
4.5584	In $_3$ Tm	4.917	EuPb $_3$
4.5644	ErIn $_3$	4.929	Ce $_3$ Sn
4.5667	CsI	4.941	LaPb $_3$
4.5732	HoIn $_3$	4.96	In $_3$ Th
4.5791	DyIn $_3$	4.964	Ce $_3$ Pb
4.588	In $_3$ U	5.011	Ce $_3$ Tl
4.5897	In $_3$ Tb	5.023	Ce $_3$ In
4.5935	In $_3$ Y	5.159	Ba(Pb $_{0.91}$ Bi $_{0.09}$ ) $_3$
4.601	GdIn $_3$	5.21	CsCdCl $_3$
4.6103	GdIn $_3$	5.29	Cs $_2$ AgAuCl $_6$
4.613	Tl $_3$ Yb	5.34	CsCdBr $_3$
4.614	In $_3$ Yb	5.45	CsHgCl $_3$
4.622	In $_3$ Sm	5.475	CsGeCl $_3$
4.6259	In $_3$ Sm	5.52	CuFeSe $_2$
4.63	Sn $_3$ U	5.559	CsPbCl $_3$
4.653	LuTl $_3$	5.655	NaY $_3$ F $_{10}$
4.655	In $_3$ Nd	5.74	NH $_4$ Tm $_3$ F $_{10}$
4.657	Tl $_3$ Tm	5.78	NH $_4$ Er $_3$ F $_{10}$
4.661	ErTl $_3$	5.78	CsHgBr $_3$
4.666	HoTl $_3$	5.81	NH $_4$ Ho $_3$ F $_{10}$
4.670	In $_3$ Pr	7.639	Ca $_3$ Al $_2$ $\theta_6$
4.671	CsI $\theta_3$	7.8	MgSr $_2$ W $\theta_6$
4.6716	In $_3$ Pr	7.80	Nb $_3$ $\theta_5$
4.6720	DyTl $_3$	7.9	Sr $_2$ ZnW $\theta_6$
4.675	Tl $_3$ U	8.0	Ca $_2$ ZnW $\theta_6$
4.6775	GdSn $_3$	8.0	CoPb $_2$ W $\theta_6$
4.680	TbTl $_3$	8.0	MgPb $_2$ W $\theta_6$
4.680	Tl $_3$ Y	8.001	Mg $_2$ PbW $\theta_6$
4.6814	Sn $_3$ Yb	8.07	BaSrZnW $\theta_6$
4.6866	SmSn $_3$	8.1	Ca $_2$ SrW $\theta_6$
4.688	CeIn $_3$	9.5852	BaH $\theta_{11}$
4.690	GdTl $_3$	9.911	Rh $_{17}$ S $_{15}$
4.696	GdTl $_3$	10.606	Pd $_{17}$ Se $_{15}$
4.6972	In $_3$ Th	12.26	Ca(AlSi $\theta_4$ ) $_2$ •5H $_2$ $\theta$
4.7060	NdSn $_3$	12.32	NaAlSi $\theta_4$ •2•3H $_2$ $\theta$
4.708	SmTl $_3$	15.43	AgCu $_3$ Pb $_3$ $\theta_3$ Cl $_7$ •3H $_2$ $\theta$
4.713	PrSn $_3$	21.87	Cu $_{12}$ Fe $_2$ S $_9$
4.721	CeSn $_3$	24.596	Na $_{12}$ Al $_{12}$ Si $_{12}$ $\theta_{48}$ •NaAl $\theta_2$ •29H $_2$ $\theta$
4.7215	Sn $_3$ Th		
Organic			
3.869	AlMn $_3$ C	4.29	CsCN
3.9249	Mn $_3$ ZnC	7.67	AgCl $\theta_4$ •3C $_4$ H $_8$ $\theta_2$
3.994	TLCN		

$\frac{4}{m} \frac{3}{m} \frac{2}{m}$	Pn3n	$O_h^2$	No. 222	Inorganic - 0	Organic - 0
.....					
$\frac{4}{m} \frac{3}{m} \frac{2}{m}$	Pm3n	$O_h^3$	No. 223	Inorganic - 72	Organic - 8
Inorganic					
4.161	UH <sub>3</sub>		5.033	PtTi <sub>3</sub>	
4.544	Cr <sub>3</sub> θ		5.048	W	
4.559	Cr <sub>3</sub> Si		5.096	AuTi <sub>3</sub>	
4.564	Cr <sub>3</sub> Si		5.115	Nb <sub>3</sub> Rh	
4.620	AsCr <sub>3.65</sub>		5.121	Nb <sub>3</sub> θs	
4.623	Cr <sub>3</sub> Ge		5.131	IrNb <sub>3</sub>	
4.656	Cr <sub>3</sub> Rh		5.153	Nb <sub>3</sub> Pt	
4.668	Cr <sub>3</sub> Ir		5.168	GeNb <sub>3</sub>	
4.675	CoV <sub>3</sub>		5.17	AlNb <sub>3</sub>	
4.6779	Cr <sub>3</sub> θs		5.1743	GeNb <sub>3</sub>	
4.6806	Cr <sub>3</sub> θs		5.1888	HgTi <sub>3</sub>	
4.683	Cr <sub>3</sub> Ru		5.21	AuNb <sub>3</sub>	
4.687	Cr <sub>3</sub> In		5.2186	SbTi <sub>3</sub>	
4.69	Cr <sub>3</sub> θs		5.2643	Nb <sub>3</sub> Sb	
4.706	Cr <sub>3</sub> Pt		5.2646	SbTa <sub>3</sub>	
4.71	NiV <sub>3</sub>		5.270	Nb <sub>3</sub> Pb	
4.722	V <sub>3</sub> Si		5.276	SnTa <sub>3</sub>	
4.75	AsV <sub>3</sub>		5.2887	Nb <sub>3</sub> Sn	
4.767	RhV <sub>3</sub>		5.48	AuZr <sub>3</sub>	
4.768	GeV <sub>3</sub>		5.4824	AuZr <sub>3</sub>	
4.7854	IrV <sub>3</sub>		5.5583	HgZr <sub>3</sub>	
4.808	PtV <sub>3</sub>		5.689	NaPt <sub>3</sub> θ <sub>4</sub>	
4.88	AuV <sub>3</sub>		5.746	CaPd <sub>3</sub> θ <sub>4</sub>	
4.890	Mo <sub>3</sub> Si		6.6444	UH <sub>3</sub>	
4.910	SiW <sub>3</sub>		6.67	F <sub>2</sub>	
4.9330	GeMo <sub>3</sub>		6.83	θ <sub>2</sub>	
4.9335	SbV <sub>3</sub>		7.562	CaNa <sub>4</sub> (Siθ <sub>3</sub> ) <sub>3</sub>	
4.937	PbV <sub>3</sub>		7.903	AuZn <sub>3</sub>	
4.94	SnV <sub>3</sub>		10.19	Na <sub>8</sub> Si <sub>4</sub> 6	
4.943	CdV <sub>3</sub>		11.92	Xe•6H <sub>2</sub> θ	
4.952	Mo <sub>3</sub> Zr		12.00	Cl <sub>2</sub> •6H <sub>2</sub> θ	
4.963	Mo <sub>3</sub> θs		12.04	Li <sub>2</sub> Na(AlSiθ <sub>4</sub> ) <sub>3</sub> •6H <sub>2</sub> θ	
4.964	IrMo <sub>3</sub>		12.05	Sθ <sub>2</sub> •6H <sub>2</sub> θ	
4.987	Mo <sub>3</sub> Pt		12.33	Na <sub>0.2</sub> Tl <sub>0.8</sub> AlSiθ <sub>4</sub> •1.667H <sub>2</sub> θ	
5.0101	IrTi <sub>3</sub>		12.38	AgAlSiθ <sub>4</sub> •2H <sub>2</sub> θ	
5.019	Moθ		16.07	Hg <sub>4</sub> Cl <sub>2</sub> θ	
Organic					
11.97	C <sub>8</sub> H <sub>14</sub> θ		12.2	CCl <sub>4</sub> •12H <sub>2</sub> θ	
12.03	6.4C <sub>2</sub> H <sub>4</sub> θ•46H <sub>2</sub> θ		12.2	CHCl <sub>3</sub> •12H <sub>2</sub> θ	
12.2	C <sub>2</sub> H <sub>5</sub> Cl•12H <sub>2</sub> θ		12.33	C <sub>9</sub> H <sub>16</sub> θ	
12.2	CH <sub>2</sub> Cl <sub>2</sub> •12H <sub>2</sub> θ		15.17	C <sub>6</sub> (NH <sub>2</sub> ) <sub>6</sub>	
$\frac{4}{m} \frac{3}{m} \frac{2}{m}$	Pn3m	$O_h^4$	No. 224	Inorganic - 40	Organic - 1
Inorganic					
3.30	H <sub>2</sub> θ		8.135	CaSn(θH) <sub>6</sub>	
4.261	Cu <sub>2</sub> θ		11.596	K <sub>3</sub> (Pθ <sub>4</sub> )(Moθ <sub>3</sub> ) <sub>12</sub> •4H <sub>2</sub> θ	
4.728	Ag <sub>2</sub> θ		11.62	Tl <sub>3</sub> PMo <sub>12</sub> θ <sub>40</sub> •4H <sub>2</sub> θ	
4.816	Agθ		11.666	(NH <sub>4</sub> ) <sub>3</sub> PMo <sub>12</sub> θ <sub>40</sub> •4H <sub>2</sub> θ	
5.020	Au <sub>2</sub> S		11.70	(NH <sub>4</sub> ) <sub>3</sub> PMo <sub>12</sub> θ <sub>40</sub> •4H <sub>2</sub> θ	
5.39	Pb <sub>2</sub> θ		11.72	K <sub>3</sub> AsMo <sub>12</sub> θ <sub>40</sub> •4H <sub>2</sub> θ	
5.536	Bi <sub>2</sub> θ <sub>3</sub>		11.72	K <sub>3</sub> PMo <sub>12</sub> θ <sub>40</sub> •4H <sub>2</sub> θ	
5.69	P <sub>2</sub> Zn <sub>3</sub>		11.74	K <sub>3</sub> PW <sub>12</sub> θ <sub>40</sub> •4H <sub>2</sub> θ	
5.74	C <sub>2</sub> Ca		11.74	Tl <sub>3</sub> AsMo <sub>12</sub> θ <sub>40</sub> •4H <sub>2</sub> θ	
5.93	Mg <sub>3</sub> P <sub>2</sub>		11.801	Cs <sub>3</sub> HSiW <sub>12</sub> θ <sub>40</sub> •nH <sub>2</sub> θ	
6.07	Cd <sub>3</sub> P <sub>2</sub>		11.81	Cs <sub>3</sub> H <sub>5</sub> W <sub>12</sub> θ <sub>40</sub> •nH <sub>2</sub> θ	
6.11	As <sub>2</sub> Mg <sub>3</sub>		11.82	(NH <sub>4</sub> ) <sub>3</sub> AsMo <sub>12</sub> θ <sub>40</sub> •4H <sub>2</sub> θ	
6.30	As <sub>2</sub> Cd <sub>3</sub>		11.84	K <sub>3</sub> AsW <sub>12</sub> θ <sub>40</sub> •4H <sub>2</sub> θ	
7.77	MgSn(θH) <sub>6</sub>		11.85	(NH <sub>4</sub> ) <sub>3</sub> PW <sub>12</sub> θ <sub>40</sub> •4H <sub>2</sub> θ	
7.78	CoSn(θH) <sub>6</sub>		11.854	Cs <sub>3</sub> PW <sub>12</sub> θ <sub>40</sub> •nH <sub>2</sub> θ	
7.79	FeSn(θH) <sub>6</sub>		11.856	Cs <sub>3</sub> H <sub>2</sub> BW <sub>12</sub> θ <sub>40</sub> •nH <sub>2</sub> θ	
7.88	MnSn(θH) <sub>6</sub>		11.91	Tl <sub>3</sub> PW <sub>12</sub> θ <sub>40</sub> •4H <sub>2</sub> θ	

Pn3m  $O_h^4$  No. 224 (continued)

## Inorganic (continued)

11.94	$(NH_4)_3AsW_{12}O_{40} \cdot 4H_2O$	12.13	$H_4Si(W_3O_{10})_4 \cdot 5H_2O$
11.94	$Tl_3AsW_{12}O_{40} \cdot 4H_2O$	12.15	$H_6[H_2(W_3O_{10})_4] \cdot 5H_2O$
12.13	$H_5B(W_3O_{10})_4 \cdot 5H_2O$	12.166	$H_3PW_{12}O_{40} \cdot 5H_2O$

## Organic

5.74 CaC<sub>2</sub>

$\frac{4}{m} \frac{3}{m} \frac{2}{m}$

Fm3m  $O_h^5$  No. 225

Inorganic - 991  
Organic - 66

## Inorganic

2.910	FeV	4.34	CuH
3.52394	Ni	4.3768	$Cd_xZr_{1-x}$
3.560	(Fe, Ni)	4.378	Ag <sub>3</sub> N
3.561	Co	4.392	NNb
3.595	C <sub>x</sub> Fe	4.40	Nb
3.608	(Fe, Ni, P)	4.404	Li
3.61529	Cu	4.406	TiH
3.6468	Fe	4.41	NSc
3.71	(Cu, Al, Mn)	4.42	NNb
3.7527	AuCu <sub>3</sub>	4.422	TaO
3.8033	Rh	4.440	TiD <sub>1.971</sub>
3.824	(Ir, Au, Os)	4.445	MnO
3.8389	Ir	4.446	Ne
3.8493	(Ir, Os)	4.45	NSc
3.8605	CrH <sub>2</sub>	4.454	CTa
3.8902	Pd	4.4662	CNb
3.9237	Pt	4.477	MnO
3.96	Al <sub>2</sub> O <sub>3</sub>	4.50	C(Nb, V, Zr)
4.0262	LiF	4.51	CSc
4.04960	Al	4.53	Ne
4.0684	LiD	4.541	Sc
4.073	LiD	4.55	NbH <sub>2</sub>
4.07897	Au	4.5755	NZr
4.080	(Ag, Au)	4.628	Li <sub>2</sub> O
4.0834	LiH	4.628	NaF
4.0862	Ag	4.6370	Pu
4.09	VO	4.638	CHf
4.093	LiH	4.64	NZr
4.093	VO	4.641	CHf
4.11	NiO	4.65	BZr
4.12	VO	4.670	BBe <sub>2</sub>
4.13	NW	4.673	Zr <sub>4</sub> H
4.137	NV	4.676	Li <sub>9</sub> SiN <sub>3</sub> O <sub>2</sub>
4.14	NV	4.678	CZr
4.148	CrN	4.68	Hg <sub>5</sub> Tl <sub>2</sub>
4.149	C <sub>3</sub> V <sub>4</sub>	4.680	HfD <sub>1.628</sub>
4.169	CV	4.6953	CdO
4.17	Li <sub>2</sub> TiO <sub>3</sub>	4.696	CZr
4.17	TiO	4.708	CdO
4.1768	NiO	4.748	Li <sub>9</sub> GeN <sub>3</sub> O <sub>2</sub>
4.212	Li <sub>3</sub> NbO <sub>4</sub>	4.759	NaTiO <sub>2</sub>
4.213	MgO	4.760	Li <sub>9</sub> TiN <sub>3</sub> O <sub>2</sub>
4.214	Li <sub>3</sub> TaO <sub>4</sub>	4.766	LuN
4.23	NTi	4.768	ZrD <sub>2</sub>
4.24	CV	4.78315	SCH <sub>2</sub>
4.2419	NTi	4.786	NYb
4.243	NTi	4.809	NTm
4.244	TiO	4.812	CaO
4.244	NTi	4.83	Na <sub>2</sub> CeO <sub>3</sub>
4.251	(N, C)Ti	4.839	ErN
4.2581	CoO	4.84	Ce
4.280	ZnO	4.85	Na <sub>2</sub> PrO <sub>3</sub>
4.29	FeO	4.851	Tl
4.29	NV	4.86	YbO
4.299	FeO	4.874	HoN
4.306	Co	4.877	NY
4.31	CV	4.882	NaH
4.321	(C, Fe, Ti)Ti	4.889	NU
4.3276	CTi	4.890	NaH
4.34	Be <sub>2</sub> C	4.897	NNp

Fm3m  $O_h^5$  No. 225 (continued)

## Inorganic (continued)

4.905	DyN	5.344	KF
4.905	NPu	5.350	Na
4.920	CPu	5.355	ErPa $\delta_4$
4.93	AgF	5.356	CoSi $_2$
4.93	U $\delta$	5.359	PuH $_2$
4.933	NTb	5.361	YPa $\delta_4$
4.9496	Pb	5.362	HoPa $\delta_4$
4.958	Pu $\delta$	5.363	Y $\delta$ F
4.9598	CU	5.365	CoSi $_2$
4.96	Am $\delta$	5.37	Pr $\delta_2$
4.961	Pa $\delta$	5.372	Cm $\delta_2$
4.961	CU	5.376	Am $\delta_2$
4.97	CPu	5.376	SmH $_2$
4.980	(LiMg)N	5.381	DyPa $\delta_4$
4.99	GdN	5.386	(Li,U) $\delta_{2+x}$
5.004	CNp	5.387	TbPa $\delta_4$
5.01	Np $\delta$	5.394	Pr $\delta_2$
5.014	EuN	5.395	NiSi $_2$
5.021	CeN	5.3960	Pu $\delta_2$
5.026	Sm $\delta$	5.40	Pr $\delta_2$
5.033	LuH $_2$	5.403	GdPa $\delta_4$
5.046	NSm	5.41	CdF $_2$
5.047	Li $_2$ NH	5.412	EuPa $\delta_4$
5.081	(MgZr $_3$ ) $\delta_7$	5.412	TmS
5.083	Sr $\delta$	5.416	Ce $\delta_2$
5.0847	Th	5.416	Sc $_2$ Se $_3$
5.09	Th	5.42	(Ce,Th) $\delta_2$
5.09	Zr $\delta_2$	5.422	SmPa $\delta_4$
5.090	TmH $_2$	5.43	CmPa $\delta_4$
5.114	Sr $\delta$	5.432	CaCdNaYF $_8$
5.123	ErH $_2$	5.4341	Np $\delta_2$
5.1233	Ce	5.44	Pb $\delta_{2-x}$
5.125	Hf $\delta_2$	5.443	PuPa $\delta_4$
5.13	CaNH	5.455	CePa $\delta_4$
5.130	CeC	5.455	U $\delta_2$
5.1396	Sr $\delta$	5.458	AmPa $\delta_4$
5.13988	LiCl	5.458	NdPa $\delta_4$
5.1426	Eu $\delta$	5.459	MnSe
5.151	NdN	5.46	Pa $\delta_{2.2}$
5.153	Ce	5.46	SrNE
5.153	LiCl	5.462	CaF $_2$
5.161	Pr	5.463	MgSe
5.165	HoH $_2$	5.463	Na $_5$ Lu $_9$ F $_{32}$
5.165	NPr	5.466	YS
5.17	CaNH	5.4691	U $\delta_2$
5.17	La	5.470	NdH $_2$
5.201	DyH $_2$	5.471	PrPa $\delta_4$
5.2034	MgS	5.471	Na $_5$ Yb $_9$ F $_{32}$
5.205	YH $_2$	5.477	HCl
5.223	MnS	5.479	AgLuS $_2$
5.246	TbH $_2$	5.484	US
5.251	ZrS	5.4862	Yb
5.256	Zr $\delta_2$	5.490	Na $\delta_2$
5.257	ScPa $\delta_4$	5.491	AgYbS $_2$
5.261	Po $_{0.9}$ Zr	5.493	Na $_5$ Tm $_9$ F $_{32}$
5.28	InPa $\delta_4$	5.50	Cu $_5$ FeS $_4$
5.286	LaN	5.501	LiBr
5.289	Tb $_4\delta_7$	5.501	AgTmS $_2$
5.295	LaN	5.505	Pa $\delta_2$
5.30	CdS	5.512	AgErS $_2$
5.30	Hf $\delta_2$	5.514	AsIn
5.303	GdH $_2$	5.514	Na $_5$ Er $_9$ F $_{32}$
5.303	N $_{1.80}$ U	5.516	PrH $_2$
5.307	La	5.517	PrH $_2$
5.31081	Ar	5.518	NaGdF $_4$
5.311	Ac	5.519	Sm $\delta$ F
5.312	FSc	5.525	LaPa $\delta_4$
5.32	N $_2$ U	5.533	LuP
5.322	LuPa $\delta_4$	5.536	PuS
5.323	LuS	5.537	Na $_5$ Ho $_9$ F $_{32}$
5.331	YbPa $\delta_4$	5.539	(Pb,Th,U) $\delta_2$
5.339	TmPa $\delta_4$	5.54	CdSe
5.34	CTh	5.54	NaH

Fm3m  $O_h^5$  No. 225 (continued)

## Inorganic (continued)

5.542	BaO	5.780	AsU
5.546	Ir <sub>2</sub> P	5.79	KOH
5.547	Na <sub>5</sub> Dy <sub>9</sub> F <sub>32</sub>	5.794	SrF <sub>2</sub>
5.549	Mo <sub>3</sub> O	5.808	EuF <sub>2</sub>
5.55	HgF <sub>2</sub>	5.817	Sc <sub>2</sub> Te <sub>3</sub>
5.556	AgCl	5.82	AlCu <sub>3</sub>
5.56	Na <sub>2</sub> O	5.830	PTh
5.573	PTm	5.8343	PTh
5.574	GdS	5.838	NdP
5.575	Cu <sub>1.8</sub> S	5.84	InSb
5.575	Na <sub>5</sub> Tb <sub>9</sub> F <sub>32</sub>	5.85	BaNH
5.576	LuSe	5.852	NaBiSe <sub>2</sub>
5.576	Na <sub>2</sub> UF <sub>6</sub>	5.854	LaS
5.58	LiBiS <sub>2</sub>	5.854	Li <sub>5</sub> P <sub>3</sub> Si
5.581	CeH <sub>2</sub>	5.855	AsPu
5.582	Ca	5.86	BiSe
5.584	ThO <sub>2</sub>	5.863	SmS
5.592	NaSmF <sub>4</sub>	5.87	TlSbS <sub>2</sub>
5.594	Na <sub>5</sub> Gd <sub>9</sub> F <sub>32</sub>	5.872	PPr
5.595	NdOF	5.879	YbSe
5.600	Pb(UO <sub>2</sub> )O <sub>2</sub>	5.88	NaCN
5.600	PU	5.89	GeLi <sub>5</sub> P <sub>3</sub>
5.602	LaH <sub>3</sub>	5.890	Pb <sub>0.33</sub> Bi <sub>0.66</sub> F <sub>2.66</sub>
5.61	PoBr <sub>4</sub>	5.891	NdSe
5.626	Ag(Cl, Br)	5.892	Cu <sub>2</sub> GeLi
5.627	Na <sub>5</sub> Eu <sub>9</sub> F <sub>32</sub>	5.900	CoMnSb
5.627	Na <sub>5</sub> Sm <sub>9</sub> F <sub>32</sub>	5.903	MnNiSb
5.63	(ThO <sub>2</sub> H) <sub>2</sub>	5.906	KCeF <sub>4</sub>
5.637	PoO <sub>2</sub>	5.909	NdSe
5.64	RbF	5.912	AgAsZn
5.640	TmSe	5.912	AsNaZn
5.6402	NaCl	5.913	Pb <sub>0.66</sub> Bi <sub>0.33</sub> F <sub>2.33</sub>
5.644	PPu	5.92	PbS
5.644	PrOF	5.92	AlCu <sub>2</sub> Mn
5.654	Bi <sub>4</sub> MoO <sub>9</sub>	5.92	Cu <sub>2</sub> NiSn
5.654	NaNdF <sub>4</sub>	5.921	AsSm
5.658	LaH <sub>2</sub>	5.922	Al <sub>2</sub> Pt
5.66	CeOF	5.922	KBiSe <sub>2</sub>
5.661	PY	5.923	Co <sub>2</sub> GaTa
5.667	LaH <sub>2</sub>	5.923	Ga <sub>2</sub> Pt
5.670	Co <sub>2</sub> MnSi	5.924	AsLiZn
5.675	Na <sub>5</sub> Nd <sub>9</sub> F <sub>32</sub>	5.924	CaSe
5.680	AsLu	5.927	AlCo <sub>2</sub> Ta
5.682	ThS	5.933	GaNi <sub>2</sub> Ta
5.687	Na <sub>2</sub> ThF <sub>6</sub>	5.93935	PbF <sub>2</sub>
5.690	PbAg <sub>4</sub> Bi <sub>4</sub> S <sub>9</sub>	5.94	PbS
5.693	NdS	5.943	AcOF
5.697	CaS	5.944	KLaF <sub>4</sub>
5.70	GeMn <sub>y</sub> Ni <sub>x</sub>	5.945	GaHfNi <sub>2</sub>
5.706	Kr	5.946	AlCo <sub>2</sub> Nb
5.71	PuOF	5.946	K <sub>2</sub> UF <sub>6</sub>
5.710	InP	5.947	PrSe
5.710	KH	5.949	AlNi <sub>2</sub> Ta
5.712	KH	5.95	Li <sub>2</sub> Se
5.720	Li <sub>2</sub> S	5.952	PrSe
5.721	AsTm	5.953	Li <sub>5</sub> P <sub>3</sub> Ti
5.728	AsSn	5.954	Co <sub>2</sub> GaNb
5.740	Cu <sub>2-x</sub> Se	5.958	GaNbNi <sub>2</sub>
5.745	Co <sub>2</sub> GeMn	5.961	LuTe
5.747	PrS	5.969	EuS
5.751	USe	5.97	CuGeLi <sub>2</sub>
5.7594	Cu <sub>1.80</sub> Se	5.97	PbS
5.760	Cu <sub>2</sub> Se	5.970	EuS
5.760	FSm	5.970	AsNd
5.763	CeS	5.972	AsTh
5.766	AsU	5.974	AlNbNi <sub>2</sub>
5.768	LaOF	5.974	NaBr
5.77	NaBiS <sub>2</sub>	5.98	(Cr, Ni)Cu <sub>2</sub> Sn
5.772	GdSe	5.98	CoCu <sub>2</sub> Sn
5.775	NaBiS <sub>2</sub>	5.982	CeSe
5.776	AgBr	5.992	CeSe
5.776	Cu <sub>2</sub> LiSi	5.992	GeTe
5.778	CeS	5.998	GeTe
5.78	HBr	6.002	CsF

Fm3m  $0_h^5$  No. 225 (continued)

## Inorganic (continued)

6.003	Co <sub>2</sub> MnSn	6.2919	AgAuZn <sub>2</sub>
6.006	K <sub>2</sub> ThF <sub>6</sub>	6.29294	KCl
6.009	AlCo <sub>2</sub> Hf	6.2956	AgAuZn <sub>2</sub>
6.009	AsPr	6.298	SnTe
6.01	Al <sub>2</sub> Au	6.30	TlCl
6.01	Cu <sub>3</sub> Sb	6.31	NaSeH
6.012	LiI	6.318	SbTh
6.017	Li <sub>2</sub> Se	6.32	NdSb
6.02	KBiS <sub>2</sub>	6.322	NdSb
6.020	SrS	6.322	PrTe
6.042	KBiS <sub>2</sub>	6.338	IrSn <sub>2</sub>
6.046	GeTh	6.353	YbTe
6.048	MgNiSb	6.356	BiU
6.049	RbH	6.358	CaTe
6.049	TmTe	6.359	CeTe
6.051	InMnNi <sub>2</sub>	6.36	PbTe
6.0555	LuSb	6.36	KHF <sub>2</sub>
6.059	Co <sub>2</sub> SnTi	6.362	BiSm
6.060	LaSe	6.366	In <sub>2</sub> Pt
6.066	CuMnSb	6.366	PrSb
6.072	AsCe	6.381	BaS
6.075	AuGa <sub>2</sub>	6.381	RaF <sub>2</sub>
6.08	Cu <sub>2</sub> MnSn	6.387	GeMg <sub>2</sub>
6.08	NaSH	6.3875	BaS
6.081	AlCo <sub>2</sub> Zr	6.389	CsH
6.081	AlH <sub>2</sub> Ni <sub>2</sub>	6.391	GeMg <sub>2</sub>
6.087	Sr	6.395	RbNH <sub>2</sub>
6.091	SbTm	6.404	Mg <sub>2</sub> Si
6.10	ErSb	6.41	CeSb
6.10	HoSb	6.41	GeHgLi <sub>2</sub>
6.115	KNH <sub>2</sub>	6.412	CeSb
6.122	PbSe	6.42	BiNd
6.123	AlNi <sub>2</sub> Zr	6.42	CdGeLi <sub>2</sub>
6.1263	In( Te, Sb )	6.42	AuLi <sub>2</sub> Sn
6.1265	PbSe	6.422	LaTe
6.1273	AuCuZn <sub>2</sub>	6.425	PtSn <sub>2</sub>
6.128	In <sub>4</sub> ( SbTe <sub>3</sub> )	6.436	LaTe
6.13	DySb	6.443	PbTe
6.137	AsLa	6.449	K <sub>2</sub> O
6.14	GeLi <sub>2</sub> Zn	6.452	PbTe
6.142	SbSn	6.461	BiPr
6.147	PbSe	6.475	NaI
6.153	InMgNi <sub>2</sub>	6.48	Li <sub>2</sub> Te
6.156	BiLu	6.488	LaSb
6.16	SbTb	6.49	LaSb
6.160	InTe	6.500	BiCe
6.163	UTe	6.51	KCN
6.164	CuMgSb	6.515	AuIn <sub>2</sub>
6.166	BiMgNi	6.517	Li <sub>2</sub> Te
6.171	SmSe	6.539	Na <sub>2</sub> S
6.172	AlCu <sub>2</sub> Hf	6.547	NH <sub>4</sub> Cl
6.176	SbU	6.57	AgLi <sub>2</sub> Sn
6.18	TlBiSe <sub>2</sub>	6.578	BiLa
6.183	PuTe	6.58	TlBr
6.185	EuSe	6.585	EuTe
6.1865	Cu <sub>2</sub> InMn	6.590	RbCl
6.19	HI	6.594	SmTe
6.19	Xe	6.599	KBr
6.190	EuSe	6.660	SrTe
6.191	SbU	6.68	KSH
6.192	BiTm	6.687	Li <sub>3</sub> Pb
6.196	BaF <sub>2</sub>	6.756	Rb <sub>2</sub> O
6.20	BiDy	6.759	Mg <sub>2</sub> Sn
6.200	SmSe	6.76	N <sub>2</sub> H <sub>4</sub> •H <sub>2</sub> O
6.2023	Xe	6.7630	Mg <sub>2</sub> Sn
6.21	BiTb	6.77	Mg <sub>2</sub> Pb
6.215	AlCu <sub>2</sub> Zr	6.779	Mg <sub>2</sub> Sn
6.22	BiEr	6.813	Mg <sub>2</sub> Pb
6.23	BiHo	6.823	Na <sub>2</sub> Se
6.246	SrSe	6.850	Mg <sub>2</sub> Pb
6.250	Xe	6.868	RbBr
6.26	CuLi <sub>2</sub> Sn	6.91	NH <sub>4</sub> Br
6.262	NdTe	6.93	KSeH
6.271	SbSm	6.94	CsCl



Fm3m  $O_h^5$  No. 225 (continued)

## Inorganic (continued)

6.94	TlI	8.463	Rb <sub>2</sub> SiF <sub>6</sub>
6.96	BaCd <sub>3</sub>	8.467	Tl <sub>2</sub> VF <sub>5</sub> •H <sub>2</sub> O
6.98	RbSH	8.476	CaPbF <sub>6</sub>
6.99	SrCl <sub>2</sub>	8.49	Ba <sub>2</sub> ScUO <sub>6</sub>
7.000	BaTe	8.49	Rb <sub>2</sub> TiF <sub>6</sub>
7.029	RbBH <sub>4</sub>	8.493	K <sub>3</sub> Sh
7.06555	KI	8.52	Ba <sub>2</sub> MnUO <sub>6</sub>
7.09	CsCl	8.521	Ba <sub>2</sub> InUO <sub>6</sub>
7.22	RbSeH	8.54	K <sub>3</sub> CrF <sub>6</sub>
7.23	CsBr	8.55	K <sub>3</sub> AlF <sub>6</sub>
7.259	NH <sub>4</sub> I	8.55	K <sub>3</sub> CoF <sub>6</sub>
7.31	GdMg <sub>3</sub>	8.551	Ba <sub>2</sub> InUO <sub>5.5</sub>
7.329	Na <sub>2</sub> Te	8.56	K <sub>3</sub> CoF <sub>7</sub>
7.340	RbI	8.57	Ba <sub>2</sub> SrWO <sub>6</sub>
7.36	K <sub>2</sub> S	8.57	Rb <sub>2</sub> PdF <sub>6</sub>
7.408	B <sub>12</sub> Zr	8.58	K <sub>3</sub> FeF <sub>6</sub>
7.419	CsBH <sub>4</sub>	8.580	Tl <sub>2</sub> SiF <sub>6</sub>
7.422	B <sub>12</sub> Sc	8.62	Ba <sub>2</sub> LaTaO <sub>6</sub>
7.52	AgPF <sub>6</sub>	8.62	Ba <sub>3</sub> WO <sub>6</sub>
7.61	NaPF <sub>6</sub>	8.66	BaSr <sub>2</sub> UO <sub>6</sub>
7.66	CsI	8.69	Ba <sub>3</sub> TaO <sub>5.5</sub>
7.67	Rb <sub>2</sub> S	8.71	Ba <sub>2</sub> CaUO <sub>6</sub>
7.692	K <sub>2</sub> Se	8.805	BiK <sub>3</sub>
7.74	KNa <sub>2</sub> Sb	8.86	Ba <sub>2</sub> SrUO <sub>6</sub>
7.74	AgAsF <sub>6</sub>	8.86	Rb <sub>3</sub> CoF <sub>6</sub>
7.75	Ca <sub>2</sub> MgWO <sub>6</sub>	8.88	Rb <sub>3</sub> AlF <sub>6</sub>
7.83	CaMgSrWO <sub>6</sub>	8.88	Rb <sub>3</sub> FeF <sub>6</sub>
7.85	Te(OH) <sub>6</sub>	8.885	Cs <sub>2</sub> SiF <sub>6</sub>
7.91	MgSr <sub>2</sub> WO <sub>6</sub>	8.89	K <sub>3</sub> NbO <sub>6</sub> F <sub>6</sub>
7.92	RbPF <sub>6</sub>	8.895	Li <sub>6</sub> NBr <sub>3</sub>
7.95	Na <sub>3</sub> AlF <sub>6</sub>	8.905	Cs <sub>2</sub> CoF <sub>6</sub>
7.978	Ca <sub>3</sub> Nb <sub>2</sub> O <sub>8</sub>	8.92	Cs <sub>2</sub> MnF <sub>6</sub>
8.02	Ca <sub>3</sub> WO <sub>6</sub>	8.92	Cs <sub>2</sub> K(CuF <sub>6</sub> )
8.066	Sr <sub>3</sub> UFe <sub>2</sub> O <sub>9</sub>	8.922	Ba <sub>3</sub> UO <sub>6</sub>
8.099	Ba <sub>2</sub> MgWO <sub>6</sub>	8.93	(NH <sub>4</sub> ) <sub>3</sub> AlF <sub>6</sub>
8.124	K <sub>2</sub> NiF <sub>6</sub>	8.94	Cs <sub>2</sub> NiF <sub>6</sub>
8.13	Na <sub>3</sub> CoF <sub>6</sub>	8.96	Cs <sub>2</sub> TiF <sub>6</sub>
8.168	K <sub>2</sub> Te	8.97	K <sub>3</sub> ZrF <sub>7</sub>
8.17	K <sub>2</sub> CrF <sub>6</sub>	8.989	BiRb <sub>3</sub>
8.184	K <sub>2</sub> SiF <sub>6</sub>	9.000	Cs <sub>2</sub> PdF <sub>6</sub>
8.20	CaSr <sub>2</sub> WO <sub>6</sub>	9.009	Cs <sub>2</sub> GeF <sub>6</sub>
8.246	K <sub>2</sub> NaGaF <sub>6</sub>	9.022	Cs <sub>2</sub> CrF <sub>6</sub>
8.250	Ba(U <sub>1/3</sub> F <sub>2/3</sub> ) <sub>3</sub> O <sub>3</sub>	9.08	Cs <sub>2</sub> Rb(CuF <sub>6</sub> )
8.266	K <sub>2</sub> NaCrF <sub>6</sub>	9.08	K <sub>3</sub> TbF <sub>7</sub>
8.27	K <sub>2</sub> (Te, Sb)	9.10	(NH <sub>4</sub> ) <sub>3</sub> FeF <sub>6</sub>
8.27	NaNbF <sub>6</sub>	9.175	Cs <sub>2</sub> K(AsF <sub>6</sub> )
8.27	NaTaF <sub>6</sub>	9.202	Rb <sub>3</sub> InF <sub>6</sub>
8.27	Sr <sub>2</sub> LaTaO <sub>6</sub>	9.210	Cu <sub>6</sub> PbO <sub>8</sub>
8.28	K <sub>2</sub> MnF <sub>6</sub>	9.22	(NH <sub>4</sub> ) <sub>3</sub> TiO <sub>2</sub> F <sub>5</sub>
8.29	BaCaSrWO <sub>6</sub>	9.22	Cs <sub>3</sub> CoF <sub>6</sub>
8.29	BaMgSrWO <sub>6</sub>	9.22	K <sub>3</sub> UF <sub>7</sub>
8.297	Ba <sub>2</sub> CrUO <sub>6</sub>	9.24	Cs <sub>3</sub> AlF <sub>6</sub>
8.312	Ba <sub>2</sub> FeUO <sub>6</sub>	9.26	(NH <sub>4</sub> ) <sub>3</sub> SCF <sub>6</sub>
8.32	K <sub>2</sub> TiF <sub>6</sub>	9.31	Rb <sub>3</sub> ZrF <sub>7</sub>
8.323	K <sub>2</sub> NaFeF <sub>6</sub>	9.310	BiCs <sub>3</sub>
8.336	Ba <sub>2</sub> NiUO <sub>6</sub>	9.384	(NH <sub>4</sub> ) <sub>3</sub> ZrF <sub>7</sub>
8.34	Sr <sub>3</sub> TaO <sub>5.5</sub>	9.42	Rb <sub>3</sub> CeF <sub>6</sub>
8.355	Ba <sub>2</sub> CaMoO <sub>6</sub>	9.45	Ca <sub>7</sub> Ge
8.374	Ba <sub>2</sub> CoUO <sub>6</sub>	9.478	Rb <sub>3</sub> PrF <sub>6</sub>
8.381	Ba <sub>2</sub> MgUO <sub>6</sub>	9.49	Rb <sub>3</sub> TbF <sub>7</sub>
8.381	Mg <sub>6</sub> MnO <sub>8</sub>	9.503	Cs <sub>3</sub> InF <sub>6</sub>
8.390	Ba <sub>2</sub> CaWO <sub>6</sub>	9.52	AgVF <sub>6</sub>
8.397	Rb <sub>2</sub> Cr(F <sub>5</sub> (H <sub>2</sub> O))	9.6445	K <sub>2</sub> MnCl <sub>6</sub>
8.397	Ba <sub>2</sub> ZnUO <sub>6</sub>	9.738	K <sub>2</sub> RuCl <sub>6</sub>
8.40	K <sub>2</sub> (Sb, Te)	9.74	K <sub>2</sub> PdCl <sub>6</sub>
8.40	(NH <sub>4</sub> ) <sub>2</sub> SiF <sub>6</sub>	9.745	K <sub>2</sub> PtCl <sub>6</sub>
8.427	Tl <sub>2</sub> (CrF <sub>5</sub> (H <sub>2</sub> O))	9.749	K <sub>2</sub> OsCl <sub>6</sub>
8.430	Rb <sub>2</sub> MnF <sub>6</sub>	9.752	K <sub>2</sub> (Pt, Rh)Cl <sub>6</sub>
8.435	K <sub>3</sub> AlF <sub>6</sub>	9.775	Tl <sub>2</sub> PtCl <sub>6</sub>
8.44	K <sub>3</sub> NiF <sub>6</sub>	9.792	K <sub>2</sub> TiCl <sub>6</sub>
8.44	Rb <sub>2</sub> VF <sub>5</sub> •H <sub>2</sub> O	9.797	Cs <sub>3</sub> TbF <sub>7</sub>
8.46	(NH <sub>4</sub> ) <sub>2</sub> GeF <sub>6</sub>	9.82	K <sub>2</sub> ReCl <sub>6</sub>
8.46	Tl <sub>2</sub> TiF <sub>6</sub>	9.82	K <sub>2</sub> TcCl <sub>6</sub>
8.462	Rb <sub>2</sub> NiF <sub>6</sub>	9.82	K <sub>2</sub> OsCl <sub>6</sub>

Fm3m  $O_h^5$  No. 225 (continued)

## Inorganic (continued)

9.825	$K_2TeCl_6$	10.240	$Cs_2TiCl_6$
9.84	$(NH_4)_2PdCl_6$	10.242	$Rb_2TeCl_6$
9.84	$Tl_2MoCl_6$	10.25	$K_2PdBr_6$
9.840	$K_2ReCl_6$	10.254	$Be_{13}Tb$
9.842	$Ag_7(OF)_3$	10.254	$Rb_2TeCl_6$
9.843	$K_2ReCl_6$	10.260	$Cs_2ReCl_6$
9.85	$K_2MoCl_6$	10.27	$Cs_2MoCl_6$
9.854	$(NH_4)_2PtCl_6$	10.27	$Cs_2WCl_6$
9.87	$Rb_2PdCl_6$	10.27	$K_2PtBr_6$
9.87	$Tl_2WCl_6$	10.27	$Rb_2PdBr_6$
9.875	$K_2WCl_6$	10.287	$Cs_2SeCl_6$
9.881	$(NH_4)_2OsCl_6$	10.29	$Ag_3(Fe(CN)_6)$
9.881	$K_2ReCl_6$	10.32	$Cu(NH_3)_6Br_2$
9.89	$(NH_4)_2IrCl_6$	10.32	$K_2OsBr_6$
9.890	$(NH_4)_2TiCl_6$	10.33	$(NH_4)_2PdBr_6$
9.890	$Ag_7N_{11}$	10.34	$Co_3[Fe(CN)_6]_2 \cdot 3H_2O$
9.904	$Rb_2PtCl_6$	10.35	$(NH_4)_2PoCl_6$
9.927	$Co_9S_8$	10.36	$Ag_3[Co(CN)_6]$
9.93	$Cu_3[Co(CN)_6]_2$	10.361	$Ni(NH_3)_6Br_2$
9.94	$K_2PdBr_6$	10.368	$Cs_2SnCl_6$
9.942	$Rb_2TiCl_6$	10.37	$(NH_4)_2PtBr_6$
9.955	$(NH_4)_2SeCl_6$	10.37	$K_2PtBr_6$
9.965	$Rb_2(TeCl_6)$	10.37	$K_2OsBr_6$
9.97	$(NH_4)_2PdBr_6$	10.371	$K_2(TcBr_6)$
9.974	$Rb_2ReCl_6$	10.38	$Rb_2PdBr_6$
9.98	$(NH_4)_2ReCl_6$	10.38	$Ag_2TiFe(CN)_6$
9.98	$K_2NiFe(CN)_6$	10.382	$K_2ReBr_6$
9.98	$K_2SnCl_6$	10.384	$K_2BrSe_6$
9.99	$Rb_2MoCl_6$	10.387	$K_2ReBr_6$
9.990	$Tl_2SnCl_6$	10.39	$Cs_2In_{0.5}Sb_{0.5}Cl_6$
9.998	$Rb_2SeCl_6$	10.39	$Rb_2TiBr_6$
10.0	$R_2CuFe(CN)_6$	10.398	$(NH_4)_2OsBr_6$
10.00	$R_2NiFe(CN)_6$	10.40	$Zn_3[Fe(CN)_6]_2 \cdot 3H_2O$
10.00	$Rb_2WCl_6$	10.41	$Cs_2Tl_{0.5}Sb_{0.5}Cl_6$
10.003	$K_2SnCl_6$	10.41	$Rb_2PtBr_6$
10.005	$(Co,Ni,Cu)Se$	10.410	$Co(NH_3)_6Br_2$
10.015	$Rb_2PdCl_6$	10.419	$K_2SeBr_6$
10.02	$Ni_2Fe(CN)_6$	10.42	$Cs_2Cd(CdCl_6)$
10.04	$Rb_2PdBr_6$	10.42	$Cs_4Zn(AuCl_6)_2$
10.05	$(Fe,Ni)_9S_8$	10.428	$Cs_2ZrCl_6$
10.058	$(NH_4)_2SnCl_6$	10.43	$(NH_4)_2TiBr_6$
10.065	$Na_6(SO_4)_2ClF$	10.431	$Co_9Se_8$
10.07	$(NH_4)_2ReCl_6$	10.437	$Cs_2PbCl_6$
10.084	$Ni(NH_3)_6Cl_2$	10.44	$Pb_3[Co(NH_3)_6]_2$
10.1	$R_2CoFe(CN)_6$	10.445	$K_2ReBr_6$
10.10	$CoK_2Fe(CN)_6$	10.460	$Rb_2(TcBr_6)$
10.119	$Rb_2SnCl_6$	10.466	$Cs_2TeCl_6$
10.120	$Co(NH_3)_6Cl_2$	10.47	$[Co(NH_3)_5H_2O]SO_4Br$
10.127	$Tl_2TeCl_6$	10.47	$Cs_2AgAuCl_6$
10.14	$Co_2Fe(CN)_6$	10.48	$(NH_4)_2SeBr_6$
10.14	$Cu_3[Fe(CN)_6]_2 \cdot 3H_2O$	10.48	$Cs_2AuAuCl_6$
10.15	$(Fe,Ni)_9S_8$	10.48	$Mn_3[Fe(CN)_6]_2 \cdot 3H_2O$
10.155	$(NH_4)_2PbCl_6$	10.484	$Al_{2.5}B_6Ni_{20.5}$
10.16	$Cu_2Mn(CN)_6$	10.485	$B_6Ni_{21}V_2$
10.168	$Fe(NH_3)_6Cl_2$	10.485	$Rb_2ReBr_6$
10.179	$Mg(NH_3)_6Cl_2$	10.486	$B_6Co_{21}V_2$
10.18	$Cs_2PdCl_6$	10.489	$Fe(NH_3)_6Br_2$
10.19	$Cs_2CrCl_5$	10.489	$Mg(NH_3)_6Br_2$
10.199	$(NH_4)_2TeCl_6$	10.490	$Rb_2ReBr_6$
10.199	$Rb_2ZrCl_6$	10.495	$B_6Mn_2Ni_{21}$
10.2	$R_2FeFe(CN)_6$	10.499	$B_6Co_{21}Ge_2$
10.20	$Co_3[Co(CN)_6]_2$	10.50	$Cs_2Bi_{0.5}Sb_{0.5}Cl_6$
10.20	$FeFe(CN)_6$	10.50	$K_2SnBr_6$
10.200	$(NH_4)_2TeCl_6$	10.50	$Rb_2MoBr_6$
10.213	$Cs_2PtCl_6$	10.50	$Rb_2WBr_6$
10.216	$Rb_2PbCl_6$	10.505	$B_6Co_{21}Mo_2$
10.219	$Mn(NH_3)_6Cl_2$	10.506	$B_6Co_{21}W_2$
10.23	$Cs_2GeCl_6$	10.516	$Al_3B_6Co_{20}$
10.230	$Cs_2OsCl_6$	10.520	$B_6Co_{21}Nb_2$
10.24	$Cu_2Cr(CN)_6$	10.54	$(NH_4)_2NaRh(NH_3)_6$
10.24	$Cs_2MoCl_5$	10.540	$Mn(NH_3)_6Br_2$
10.24	$Cs_2NbCl_5$	10.542	$B_6Co_{20}Ti_3$
10.24	$Cs_2WCl_5$	10.546	$B_6Co_{21}Sc_2$
10.24	$Ni_3(Fe(CN)_6)_2 \cdot 3H_2O$	10.552	$Al_3B_7(Ni_{18}B_2)$

Fm3m  $O_h^5$  No. 225 (continued)

## Inorganic (continued)

10.555	$B_6Ni_{19.5}Zn_{3.5}$	11.00	$Be_{15}Co_8Hf_6$
10.557	$B_6Nb_2Ni_{21}$	11.000	$Mg(NH_3)_6I_2$
10.56	$B_6Ni_{21}Sc_2$	11.01	$Cs_2PoBr_6$
10.56	$AgTl_2Fe(CN)_6$	11.04	$B_6(Re,Co)_23$
10.56	$Sr_2Ni(NO_2)_6$	11.059	$Mn(NH_3)_6I_2$
10.569	$B_6Mg_3Ni_{20}$	11.06	$Be_{15}Ni_8Zr_6$
10.57	$Cs_2TiBr_6$	11.068	$Cd(NH_3)_6I_2$
10.57	$Pb_2Ni(NO_2)_6$	11.1	$B_6(Re,Fe)_23$
10.574	$B_6Co_{21}Hf_2$	11.10	$Be_{15}Co_8Zr_6$
10.577	$B_6Ni_{20}Ti_3$	11.10	$Cr_6Ni_{16}Si_7$
10.580	$B_6Co_{21}In_2$	11.154	$Mn_6Ni_{16}Si_7$
10.581	$B_6In_2Ni_{21}$	11.185	$Be_{15}Cu_8Zr_6$
10.582	$B_6Co_{21}Zr_2$	11.193	$B_6Mn_{11}Re_{12}$
10.59	$Ba_3[Co(NO_2)_6]_2$	11.20	$Tl_3[Co(CN)_6]$
10.594	$B_6Ni_{20}Zr_3$	11.241	$Ni(NH_3)_6(BF_4)_2$
10.598	$B_6Co_{21}Sb_2$	11.25	$B_6Ni_{11}Re_{12}$
10.598	$B_6Ni_{21}Sb_2$	11.251	$Co_{16}Nb_6Si_7$
10.598	$B_6Ni_{21}Sn_2$	11.28	$CdNa_6Cl_8$
10.60	$Rb_2SnBr_6$	11.288	$Co(NH_3)_6(BF_4)_2$
10.61	$(NH_4)_2SnBr_6$	11.301	$Rb_2(TcI_6)$
10.62	$(B,C)_6Fe_{23}$	11.31	$Rb_2ReI_6$
10.62	$Cs_2PdBr_6$	11.320	$Rb_2ReI_6$
10.620	$B_6Co_{21}U_2$	11.360	$Mg(NH_3)_6(BF_4)_2$
10.63	$Cs_2PtBr_6$	11.363	$Fe(NH_3)_6(BF_4)_2$
10.64	$[Co(NH_3)_5H_2O]SeO_4I$	11.397	$Mn(NH_3)_6(BF_4)_2$
10.649	$B_6Hf_3Ni_{20}$	11.403	$Cd(NH_3)_6(BF_4)_2$
10.65	$Cs_4Cd(AuCl_6)_2$	11.433	$Ni(NH_3)_6(ClO_4)_2$
10.65	$[Co(NH_3)_6]SeO_4Br$	11.44	$Cs_2ReI_6$
10.65	$Ag_2TlCo(CN)_6$	11.468	$Ni(NH_3)_6(SO_3F)_2$
10.652	$B_6Ni_{21}U_2$	11.472	$Co(NH_3)_6(ClO_4)_2$
10.659	$Cs_2OsBr_6$	11.513	$Co(NH_3)_6(SO_3F)_2$
10.659	$C_6Cr_{23}$	11.540	$Fe(NH_3)_6(ClO_4)_2$
10.66	$Cs_2PdBr_6$	11.554	$Mg(NH_3)_6(ClO_4)_2$
10.66	$Rb_2SnBr_6$	11.567	$Fe(NH_3)_6(SO_3F)_2$
10.67	$Cs_2PtBr_6$	11.601	$Mn(NH_3)_6(ClO_4)_2$
10.68	$Be_{15}Ni_8Ta_6$	11.611	$Cd(NH_3)_6(ClO_4)_2$
10.68	$Cd_3[Fe(CN)_6]_2 \cdot 3H_2O$	11.616	$Mn(NH_3)_6(SO_3F)_2$
10.68	$Cs_4Hg(AuCl_6)_2$	11.62	$Rb_2SnI_6$
10.685	$Cs_2ReBr_6$	11.642	$Cd(NH_3)_6(SO_3F)_2$
10.69	$Ba_2Ni(NO_2)_6$	11.65	$Cs_2SnI_6$
10.70	$Cs_2MoBr_6$	11.67	$Cu_{16}Mg_6Si_7$
10.70	$Cs_2WBr_6$	11.722	$Cs_2TeI_6$
10.722	$Cs_2SeBr_6$	11.79	$Cs_2PoI_6$
10.728	$(NH_4)_2TeBr_6$	11.936	$Ni(NH_3)_6(PF_6)_2$
10.73	$Be_{15}Nb_6Ni_8$	11.95	$Fe_{23}Lu_6$
10.74	$Cu(NH_3)_6I_2$	11.966	$Co(NH_3)_6(PF_6)_2$
10.74	$Cu_3SbS_4$	11.98	$Fe_{23}Tm_6$
10.771	$Rb_2TeBr_6$	12.00	$Al_{15}Hf_6Ni_8$
10.775	$Be_{15}Cu_8Ta_6$	12.01	$Er_6Fe_{23}$
10.784	$Be_{15}Cu_8Ti_6$	12.04	$Fe_{23}Ho_6$
10.797	$Cs_2SnBr_6$	12.06	$Dy_6Fe_{23}$
10.81	$[Co(NH_3)_6]SeO_4I$	12.07	$Fe_{23}Tb_6$
10.82	$Co(NH_3)_6I_3$	12.08	$Al_{15}Ni_8Zr_6$
10.83	$Cs_2SnBr_6$	12.12	$Fe_{23}Y_6$
10.83	$AgTl_2Co(CN)_6$	12.21	$Lu_6Mn_{23}$
10.833	$Be_{15}Cu_8Nb_6$	12.29	$Er_6Mn_{23}$
10.84	$(NH_4)_2PoBr_6$	12.30	$Mn_{23}Tm_6$
10.897	$Ni(NH_3)_6I_2$	12.34	$Ho_6Mn_{23}$
10.90	$Cs_2HgHgCl_6$	12.38	$Dy_6Mn_{23}$
10.910	$Cs_2TeBr_6$	12.44	$Mn_{23}Tb_6$
10.918	$Cs_2TeBr_6$	12.47	$Mn_{23}Y_6$
10.93	$Cs_2AgAuBr_6$	12.51	$Gd_6Mn_{23}$
10.936	$Co(NH_3)_6I_2$	12.523	$Mn_{23}Th_6$
10.986	$Zn(NH_3)_6I_2$	12.68	$Mn_{23}Sm_6$
10.987	$Fe(NH_3)_6I_2$	14.88	$Li_{23}Sr_6$
10.99	$Be_{15}Hf_6Ni_8$	27.39	$(Fe,Al)_3Fe_4K_2H_{10}(SO_4)_{10}(OH)_9 \cdot 4H_2O$

## Organic

3.595	$FeC_x$	4.31	VC
4.149	$V_4C_3$	4.321	$Ti(C,Fe,Ti)$
4.169	VC	4.3276	TiC
4.24	VC	4.33	TiC
4.251	$Ti(N,C)$	4.34	$Be_2C$

Fm3m  $O_h^5$  No. 225 (continued)

## Organic (continued)

4.454	TaC	10.10	$CoK_2Fe(CN)_6$
4.470	NbC	10.14	$Co_2Fe(CN)_6$
4.50	(Nb, V, Zr)C	10.14	$Cu_3[Fe(CN)_6]_2 \cdot 3H_2O$
4.51	ScC	10.16	$Cu_2Mn(CN)_6$
4.638	HfC	10.2	$R_2FeFe(CN)_6$
4.641	HfC	10.20	$Co_3[Co(CN)_6]_2$
4.67	ScC <sub>0.3</sub>	10.20	$FeFe(CN)_6$
4.678	ZrC	10.24	$Cu_2Cr(CN)_6$
4.696	ZrC	10.24	$Ni_3[Fe(CN)_6]_2 \cdot 3H_2O$
4.920	PuC	10.29	$Ag_3[Fe(CN)_6]$
4.9598	UC	10.34	$Co_3[Fe(CN)_6]_2 \cdot 3H_2O$
4.97	CPu	10.36	$Ag_3[Co(CN)_6]$
5.004	NpC	10.38	$Ag_2Tl[Fe(CN)_6]$
5.34	ThC	10.40	$Zn_3[Fe(CN)_6]_2 \cdot 3H_2O$
5.88	NaCN	10.48	$Mn_3[Fe(CN)_6]_2 \cdot 3H_2O$
6.51	KCN	10.56	$AgTl_2[Fe(CN)_6]$
6.96	BaC <sub>0.3</sub>	10.62	$(C, B)_6Fe_2$
8.34	CCl <sub>4</sub>	10.65	$Ag_2Tl[Co(CN)_6]$
8.62	C <sub>4</sub> H <sub>9</sub> Cl	10.659	$Cr_2C_6$
8.78	(CH <sub>3</sub> ) <sub>4</sub> C	10.68	$Cd_3[Fe(CN)_6]_2 \cdot 3H_2O$
8.82	(CH <sub>3</sub> ) <sub>3</sub> CC <sub>0.08</sub> H	10.83	$AgTl_2[Co(CN)_6]$
9.45	C <sub>10</sub> H <sub>16</sub>	10.83	$Tl_3[Fe(CN)_6]$
9.93	$Cu_3[Co(CN)_6]_2$	11.20	$Tl_3[Co(CN)_6]$
9.98	$K_2NiFe(CN)_6$	11.84	$[(CH_3)_4N]_2B_6H_6$
10.0	$R_2CuFe(CN)_6$	12.051	$Ni(NH_2CH_3)_6I_2$
10.00	$R_2NiFe(CN)_6$	12.90	$[(CH_3)_4N]_2SnCl_6$
10.02	$Ni_2Fe(CN)_6$	13.05	$[(CH_3)_4N]_2CeCl_6$
10.1	$R_2CoFe(CN)_6$	14.34	$CaBr_2 \cdot 10H_2O \cdot 2(CH_2)_6N_4$

 $\frac{4}{m} \frac{3}{m} \frac{2}{m}$ Fm3c  $O_h^6$  No. 226Inorganic - 44  
Organic - 0

## Inorganic

10.00	Be <sub>13</sub> Hf	10.370	Be <sub>13</sub> Pr
10.005	Be <sub>13</sub> Hf	10.375	Be <sub>13</sub> Ce
10.010	Be <sub>13</sub> Hf	10.395	Be <sub>13</sub> Th
10.030	Be <sub>13</sub> Hf	10.457	Be <sub>13</sub> Sr
10.047	Be <sub>13</sub> Zr	10.460	Be <sub>13</sub> La
10.102	Be <sub>13</sub> Sc	11.85	Al <sub>6</sub> CeCu <sub>6</sub> Mn
10.166	Be <sub>13</sub> Mg	12.15	CaZn <sub>13</sub>
10.173	Be <sub>13</sub> Lu	12.216	EuZn <sub>13</sub>
10.182	Be <sub>13</sub> Yb	12.240	SrZn <sub>13</sub>
10.199	Be <sub>13</sub> Tm	12.2836	NaZn <sub>13</sub>
10.210	Be <sub>13</sub> Er	12.35	BaZn <sub>13</sub>
10.225	Be <sub>13</sub> Ho	12.360	KZn <sub>13</sub>
10.238	Be <sub>13</sub> Y	12.38	KZn <sub>13</sub>
10.239	Be <sub>13</sub> Dy	12.61	Mn
10.256	Be <sub>13</sub> Np	13.80	Cd <sub>13</sub> K
10.256	Be <sub>13</sub> U	13.91	Cd <sub>13</sub> Rb
10.283	AmBe <sub>13</sub>	13.92	Cd <sub>13</sub> Cs
10.284	Be <sub>13</sub> Pu	18.50	KTlBr <sub>4</sub> · 2H <sub>2</sub> O
10.300	Be <sub>13</sub> Eu	18.64	RbTlBr <sub>4</sub> · H <sub>2</sub> O
10.312	Be <sub>13</sub> Ca	18.85	CsTlBr <sub>4</sub>
10.325	Be <sub>13</sub> Sm	19.00	NH <sub>4</sub> TlBr <sub>4</sub> · 2H <sub>2</sub> O
10.352	Be <sub>13</sub> Nd	20.24	CsTlI <sub>4</sub>

## Organic

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 $\frac{4}{m} \frac{3}{m} \frac{2}{m}$ Fd3m  $O_h^7$  No. 227Inorganic - 651  
Organic - 21

## Inorganic

3.56	C	6.300	AgBe <sub>2</sub>
5.43035	Si	6.373	AlLi
5.65763	Ge	6.40	AlLi
5.687	NiS <sub>2</sub>	6.448	Be <sub>2</sub> Ti
6.04	Se	6.489	Sn
6.20	Be <sub>1.2</sub> Co <sub>0.8</sub> Mn	6.51	Be <sub>2</sub> Ta

Fd3m  $0_h^7$  No. 227 (continued)

## Inorganic (continued)

6.535	Be <sub>2</sub> Nb	7.2097	Co <sub>2</sub> Tb
6.589	BaSe	7.21	Cr <sub>2</sub> Zr
6.686	MnNi <sub>1.55</sub> Si <sub>0.45</sub>	7.212	Fe <sub>2</sub> Lu
6.701	CdLi	7.216	Co <sub>2</sub> Y
6.705	Co <sub>2</sub> Ti	7.226	Ni <sub>2</sub> Sm
6.706	(Co <sub>0.75</sub> Ni <sub>0.25</sub> ) <sub>3</sub> Ti	7.247	Fe <sub>2</sub> Tm
6.73	CoTi <sub>2</sub>	7.255	Co <sub>2</sub> Gd
6.733	Co <sub>2</sub> Ta	7.260	Co <sub>2</sub> Sm
6.759	Co <sub>2</sub> Nb	7.2616	Co <sub>2</sub> Sm
6.762	Ge <sub>0.5</sub> MnNi <sub>1.5</sub>	7.262	LaNi <sub>2</sub>
6.778	Co <sub>2</sub> Ta	7.270	NdNi <sub>2</sub>
6.782	Co <sub>2</sub> Nb	7.273	ErFe <sub>2</sub>
6.800	InLi	7.285	Ni <sub>2</sub> Pr
6.901	Co <sub>2</sub> Zr	7.290	Mn <sub>2</sub> Pu
6.909	Cu <sub>1.5</sub> Ga <sub>0.5</sub> Mn	7.2981	Co <sub>2</sub> Nd
6.913	Ga <sub>0.4</sub> MgNi <sub>1.6</sub>	7.300	CeFe <sub>2</sub>
6.918	Co <sub>2</sub> Hf	7.300	Fe <sub>2</sub> Ho
6.926	Ni <sub>2</sub> Sc	7.300	Co <sub>2</sub> Nd
6.927	Co <sub>2</sub> Zr	7.303	CdCuIn
6.93	Cr <sub>2</sub> Nb	7.303	CeFe <sub>2</sub>
6.94	AlCu <sub>3</sub> Mn <sub>2</sub>	7.3058	Co <sub>2</sub> Pr
6.943	Cr <sub>2</sub> Ti	7.312	InNa
6.960	Co <sub>2</sub> Zr	7.312	Co <sub>2</sub> Pr
6.960	Ni <sub>1.5</sub> V <sub>0.5</sub> Zr	7.325	DyFe <sub>2</sub>
6.961	Cr <sub>2</sub> Ta	7.343	Al <sub>1.4</sub> Ni <sub>0.6</sub> Zr
6.965	Ni <sub>2</sub> Tm	7.348	Ir <sub>2</sub> Sc
6.966	CuMnZn	7.355	Fe <sub>2</sub> Y
6.97	MgNiZn	7.359	Ir <sub>2</sub> Zr
6.979	Cr <sub>2</sub> Ta	7.369	Fe <sub>2</sub> Tb
6.990	Cr <sub>2</sub> Nb	7.378	Al <sub>1.5</sub> Co <sub>0.5</sub> Zr <sub>1.0</sub>
6.9924	Co <sub>2</sub> U	7.380	Al <sub>1.65</sub> Cu <sub>0.35</sub> Hf
7.005	Co <sub>2</sub> U	7.39	Fe <sub>2</sub> Gd
7.03	Cu <sub>2</sub> Mg	7.394	Zn <sub>2</sub> Zr
7.037	CrNiZr	7.415	Fe <sub>2</sub> Sm
7.045	MnNiZr	7.426	HoRh <sub>2</sub>
7.053	Fe <sub>2</sub> Zr	7.430	Al <sub>1.65</sub> Fe <sub>0.35</sub> Zr
7.054	FeNiU	7.442	LiMgZn
7.056	Fe <sub>2</sub> Zr	7.444	ErRh <sub>2</sub>
7.0592	Fe <sub>2</sub> U	7.459	Rh <sub>2</sub> Y
7.060	Co <sub>2</sub> Yb	7.469	NaTl
7.060	Ni <sub>2</sub> Yb	7.473	ErIr <sub>2</sub>
7.061	Fe <sub>2</sub> U	7.483	DyRh <sub>2</sub>
7.064	Cu <sub>2</sub> Mg	7.488	Rh <sub>2</sub> Y
7.065	Fe <sub>2</sub> U	7.488	NaTl <sub>2</sub>
7.075	Co <sub>2</sub> Pu	7.488	NaTl
7.083	LuNi <sub>2</sub>	7.490	HoIr <sub>2</sub>
7.09	Fe <sub>2</sub> Sc	7.500	Ir <sub>2</sub> Y
7.106	CdCu <sub>1.5</sub> Ga <sub>0.5</sub>	7.507	HoMn <sub>2</sub>
7.106	Co <sub>2</sub> Lu	7.5089	Ir <sub>2</sub> U
7.11	ErNi <sub>2</sub>	7.5124	Os <sub>2</sub> U
7.115	CdCu <sub>1.5</sub> Ge <sub>0.5</sub>	7.514	GdRh <sub>2</sub>
7.121	Co <sub>2</sub> Tm	7.524	Ir <sub>2</sub> Y
7.13	Si <sub>2</sub>	7.535	CeRu <sub>2</sub>
7.1349	Co <sub>2</sub> Tm	7.538	CeRh <sub>2</sub>
7.136	HoNi <sub>2</sub>	7.550	GdIr <sub>2</sub>
7.142	DyNi <sub>2</sub>	7.56	GdRu <sub>2</sub>
7.144	Co <sub>2</sub> Er	7.564	DyMn <sub>2</sub>
7.150	Fe <sub>2</sub> Pu	7.564	NdRh <sub>2</sub>
7.1536	Co <sub>2</sub> Er	7.571	CeIr <sub>2</sub>
7.155	DyNi <sub>2</sub>	7.5731	DyMn <sub>2</sub>
7.157	Mn <sub>2</sub> U	7.575	PrRh <sub>2</sub>
7.16	Ni <sub>2</sub> Pu	7.577	GdPt <sub>2</sub>
7.160	Ni <sub>2</sub> Tb	7.58	Mo <sub>2</sub> Zr
7.1606	CeCo <sub>2</sub>	7.580	Al <sub>2</sub> Sc
7.1628	Mn <sub>2</sub> U	7.580	Ru <sub>2</sub> Sm
7.168	Co <sub>2</sub> Ho	7.59	Mo <sub>2</sub> Zr
7.1730	Co <sub>2</sub> Ho	7.590	Pt <sub>2</sub> Y
7.181	Ni <sub>2</sub> Y	7.593	CeOs <sub>2</sub>
7.187	Co <sub>2</sub> Dy	7.5966	DyPt <sub>2</sub>
7.20	Cr <sub>2</sub> Zr	7.605	Ir <sub>2</sub> Nd
7.202	CeNi <sub>2</sub>	7.607	Pt <sub>2</sub> Y
7.202	GdNi <sub>2</sub>	7.614	NdRu <sub>2</sub>
7.206	Co <sub>2</sub> Tb	7.620	Mn <sub>2</sub> Tb
7.208	CeNi <sub>2</sub>	7.621	Ir <sub>2</sub> Pr

Fd3m  $O_h^7$  No. 227 (continued)

## Inorganic (continued)

7.624	PrRu <sub>2</sub>	8.128	NiCo <sub>2</sub> σ <sub>4</sub>
7.63	W <sub>2</sub> Zr	8.134	(Zn,Fe)(Al,Fe) <sub>2</sub> σ <sub>4</sub>
7.6349	GdPt <sub>2</sub>	8.136	FeAl <sub>2</sub> σ <sub>4</sub>
7.646	LaRh <sub>2</sub>	8.145	Al <sub>2</sub> La
7.649	Ru <sub>2</sub> Th	8.146	FeAl <sub>2</sub> σ <sub>4</sub>
7.662	Ir <sub>2</sub> Th	8.1474	Al <sub>2</sub> La
7.663	σ <sub>2</sub> Pr	8.153	Al <sub>2</sub> La
7.678	Mn <sub>2</sub> Y	8.176	Al <sub>2</sub> La
7.680	Mn <sub>2</sub> Y	8.19	LiCrMnσ <sub>4</sub>
7.686	Ir <sub>2</sub> La	8.19	Li <sub>4</sub> /3Mn <sub>5</sub> /3σ <sub>4</sub>
7.694	NdPt <sub>2</sub>	8.195	CrLi <sub>3</sub> V <sub>2</sub> σ <sub>8</sub>
7.701	LaRu <sub>2</sub>	8.21	LiGa <sub>5</sub> σ <sub>8</sub>
7.705	σ <sub>2</sub> Th	8.215	LiNiVσ <sub>4</sub>
7.709	PrPt <sub>2</sub>	8.221	Ni <sub>2</sub> Geσ <sub>4</sub>
7.723	CePt <sub>2</sub>	8.23	LiGa(Gaσ <sub>2</sub> ) <sub>4</sub>
7.724	GdMn <sub>2</sub>	8.246	LiMn <sub>2</sub> σ <sub>4</sub>
7.730	CePt <sub>2</sub>	8.252	(Mg,Fe)(Cr,Al,Fe) <sub>2</sub> σ <sub>4</sub>
7.732	GdMn <sub>2</sub>	8.255	Mg <sub>2</sub> Geσ <sub>4</sub>
7.736	Laσ <sub>2</sub>	8.258	NiGe <sub>2</sub> σ <sub>4</sub>
7.741	CePt <sub>2</sub>	8.275	Li <sub>2</sub> ZnMn <sub>3</sub> σ <sub>8</sub>
7.742	Al <sub>2</sub> Lu	8.276	CoLiVσ <sub>4</sub>
7.755	LaPt <sub>2</sub>	8.277	(Mg,Fe)(Cr,Al) <sub>2</sub> σ <sub>4</sub>
7.766	Al <sub>2</sub> U	8.28	LiGaTiσ <sub>4</sub>
7.774	LaPt <sub>2</sub>	8.280	MgGa <sub>2</sub> σ <sub>4</sub>
7.7757	Al <sub>2</sub> Tm	8.280	MnAl <sub>2</sub> σ <sub>4</sub>
7.780	Al <sub>2</sub> Tm	8.285	MnCo <sub>2</sub> σ <sub>4</sub>
7.793	Al <sub>2</sub> Er	8.286	MgGa <sub>2</sub> σ <sub>4</sub>
7.800	Pd <sub>2</sub> Sr	8.29	Co <sub>2</sub> Mnσ <sub>4</sub>
7.8031	Au <sub>2</sub> Na	8.295	(Fe,Mg)(Cr,Al) <sub>2</sub> σ <sub>4</sub>
7.811	Al <sub>2</sub> U	8.296	MgGa <sub>2</sub> σ <sub>4</sub>
7.813	Al <sub>2</sub> Ho	8.297	FeV <sub>2</sub> σ <sub>4</sub>
7.827	Al <sub>2</sub> Y	8.297	LiCrTiσ <sub>4</sub>
7.83	PbFe <sub>2</sub> σ <sub>4</sub>	8.30	CuMn <sub>2</sub> σ <sub>4</sub>
7.831	Al <sub>2</sub> Pu	8.30	LiMnTiσ <sub>4</sub>
7.8370	Al <sub>2</sub> Dy	8.30	LiRhMnσ <sub>4</sub>
7.855	Al <sub>2</sub> Y	8.301	Li <sub>2</sub> Tiσ <sub>3</sub>
7.8654	Al <sub>2</sub> Tb	8.305	(Mg,Fe)(Cr,Al) <sub>2</sub> σ <sub>4</sub>
7.877	Al <sub>2</sub> Yb	8.3070	CoGa <sub>2</sub> σ <sub>4</sub>
7.900	Al <sub>2</sub> Gd	8.313	Li <sub>2</sub> NiF <sub>4</sub>
7.91	RbAlσ <sub>2</sub>	8.316	Co <sub>1.8</sub> Mn <sub>1.2</sub> σ <sub>4</sub>
7.927	Au <sub>2</sub> Pb	8.318	Co <sub>2</sub> Geσ <sub>4</sub>
7.94	LiAl(Alσ <sub>2</sub> ) <sub>4</sub>	8.32	MgCr <sub>2</sub> σ <sub>4</sub>
7.940	Al <sub>2</sub> Sm	8.32	NiCr <sub>2</sub> σ <sub>4</sub>
7.9418	Al <sub>2</sub> Sm	8.325	CoGa <sub>2</sub> σ <sub>4</sub>
7.958	Au <sub>2</sub> Bi	8.33	CuMn <sub>2</sub> σ <sub>4</sub>
8.000	Al <sub>2</sub> Nd	8.336	CoCr <sub>2</sub> σ <sub>4</sub>
8.002	Al <sub>2</sub> Nd	8.338	NiFe <sub>2</sub> σ <sub>4</sub>
8.025	Al <sub>2</sub> Pr	8.340	ZnGe <sub>2</sub> σ <sub>4</sub>
8.0312	Al <sub>2</sub> Pr	8.340	ZnCr <sub>2</sub> σ <sub>4</sub>
8.038	Al <sub>2</sub> Ca	8.349	(Fe,Mg)(Cr,Al,Fe) <sub>2</sub> σ <sub>4</sub>
8.046	NiAl <sub>2</sub> σ <sub>4</sub>	8.359	LiFeTiσ <sub>4</sub>
8.055	CuCo <sub>2</sub> σ <sub>4</sub>	8.359	Li <sub>4</sub> Ti <sub>7</sub> σ <sub>16</sub>
8.059	Al <sub>2</sub> Ce	8.36	LiCo <sub>0.5</sub> Ti <sub>1.5</sub> σ <sub>4</sub>
8.075	CoAl <sub>2</sub> σ <sub>4</sub>	8.3630	FeGa <sub>2</sub> σ <sub>4</sub>
8.078	CdAl <sub>2</sub> σ <sub>4</sub>	8.37	CoFe <sub>2</sub> σ <sub>4</sub>
8.08	Co <sub>2</sub> Znσ <sub>4</sub>	8.37	Cu <sub>2</sub> Cr <sub>2</sub> σ <sub>4</sub>
8.080	CuAl <sub>2</sub> σ <sub>4</sub>	8.37	LiMg <sub>0.5</sub> Ti <sub>1.5</sub> σ <sub>4</sub>
8.087	ZnAl <sub>2</sub> σ <sub>4</sub>	8.37	LiZn <sub>0.5</sub> Ti <sub>1.5</sub> σ <sub>4</sub>
8.09	Co <sub>3</sub> σ <sub>4</sub>	8.372	FeCr <sub>2</sub> σ <sub>4</sub>
8.098	CsAlσ <sub>2</sub>	8.373	CuMn <sub>2</sub> σ <sub>4</sub>
8.099	(Zn,Mg)Al <sub>2</sub> σ <sub>4</sub>	8.377	MgFe <sub>2</sub> σ <sub>4</sub>
8.100	FeAl <sub>2</sub> σ <sub>4</sub>	8.382	Co <sub>2</sub> Vσ <sub>4</sub>
8.106	MgAl <sub>2</sub> σ <sub>4</sub>	8.39	CuFe <sub>2</sub> σ <sub>4</sub>
8.115	ZnAl <sub>2</sub> σ <sub>4</sub>	8.39	CuGa <sub>2</sub> σ <sub>4</sub>
8.116	MgAl <sub>2</sub> σ <sub>4</sub>	8.39	LiCu <sub>0.5</sub> Ti <sub>1.5</sub> σ <sub>4</sub>
8.12	(Mg,Fe)Al <sub>2</sub> σ <sub>4</sub>	8.39	LiFe(Feσ <sub>2</sub> ) <sub>4</sub>
8.12	Ni <sub>28</sub> σ <sub>32</sub>	8.391	CuCu <sub>2</sub> Fe(Feσ <sub>2</sub> ) <sub>8</sub>
8.12	SnAl <sub>2</sub> σ <sub>4</sub>	8.392	Feσ
8.123	MgCo <sub>2</sub> σ <sub>4</sub>	8.395	Zn <sub>2</sub> Vσ <sub>4</sub>
8.124	Co <sub>3</sub> σ <sub>4</sub>	8.397	Fe <sub>3</sub> σ <sub>4</sub>
8.124	ZnCo <sub>2</sub> σ <sub>4</sub>	8.397	Zn <sub>4</sub> V <sub>3</sub> σ <sub>10</sub>
8.125	Al <sub>2</sub> Eu	8.399	NiMn <sub>2</sub> σ <sub>4</sub>
8.126	Cr <sub>3</sub> σ <sub>4</sub>	8.403	Mg <sub>2</sub> Vσ <sub>4</sub>
8.1262	Al <sub>2</sub> Eu	8.404	NiFe <sub>2</sub> σ <sub>4</sub>

Fd3m  $O_h^7$  No. 227 (continued)

## Inorganic (continued)

8.405	$Cu_{0.5}Zn_{0.5}Fe_2\sigma_4$	8.99	$Na_2W\sigma_4$
8.407	$CuFe(Fe\sigma_2)_4$	9.108	$Na_2Mo\sigma_4$
8.410	$ZnV_2\sigma_4$	9.115	$CdIn_2\sigma_4$
8.411	$MgV_2\sigma_4$	9.1297	$Na_2W\sigma_4$
8.417	$Fe_3\sigma_4$	9.28	$Ag_2Mo\sigma_4$
8.419	$Cu_{0.4}Zn_{0.6}Fe_2\sigma_4$	9.3127	$Ag_2Mo\sigma_4$
8.419	$MnFe_2\sigma_4$	9.417	$Co_3S_4$
8.42	$FeCr_2\sigma_4$	9.43	$Co_3S_4$
8.420	$ZnFe_2\sigma_4$	9.44	$Co_{3-x}S_4$
8.422	$ZnFe_2\sigma_4$	9.446	$(Co,Ni)_3S_4$
8.425	$(Fe,Mn)Fe_2\sigma_4$	9.464	$FeNi_2S_4$
8.429	$CoFe_2\sigma_4$	9.476	$Ni_3S_4$
8.429	$Fe_3\sigma_4$	9.477	$Co_2CuS_4$
8.43	$Mg_2Ti\sigma_4$	9.48	$CuCo_2S_4$
8.431	$NiFe_2\sigma_4$	9.520	$Bi_2K$
8.433	$ZnFe_2\sigma_4$	9.601	$Bi_2Rb$
8.434	$Fe_3\sigma_4$	9.609	$Bi_2Rb$
8.4350	$MnGa_2\sigma_4$	9.630	$CuCr_2S_4$
8.4370	$(Fe,Mn)Fe_2\sigma_4$	9.746	$Bi_2Cs$
8.44	$Fe_4Ti_{0.5}\sigma_7$	9.760	$Bi_2Cs$
8.44	$ZnFe_8\sigma_{13}$	9.801	$Sc_2Ti_2\sigma_7$
8.44	$(Mn,Mg,Fe)Fe_2\sigma_4$	9.824	$CuV_2S_4$
8.44	$MnFe_2\sigma_4$	9.849	$16Al(F,\sigma H)_3 \cdot 6H_2\sigma$
8.441	$MgFe_2\sigma_4 \cdot (Mn,Fe)Fe_2\sigma_4$	9.876	$Fe_3S_4$
8.448	$Co_2Ti\sigma_4$	9.89	$(Al,Mg)_2Na_{0.35}(H_2\sigma)_{0.875}(F,\sigma H)_6$
8.449	$ZnFe_2\sigma_4$	9.90	$CrAl_2S_4$
8.457	$Mg_2Ti\sigma_4$	9.90	$CoCr_2S_4$
8.462	$CuFe_2\sigma_4$	9.91	$CoCr_2S_4$
8.462	$Zn_2Ti\sigma_4$	9.93	$Al_2S_3$
8.47	$Fe_2Ti\sigma_4$	9.933	$CuTi_2S_4$
8.477	$Zn_2Ti\sigma_4$	9.94	$Ni_3Se_4$
8.482	$ZnFe_2\sigma_4$	9.94	$ZnCr_2S_4$
8.485	$FeV_2\sigma_4$	9.945	$TiAl_2S_4$
8.495	$CoRh_2\sigma_4$	9.97	$FeCr_2S_4$
8.499	$MnFe_2\sigma_4$	9.986	$FeCr_2S_4$
8.504	$MnCr_2\sigma_4$	9.988	$ZnAl_2S_4$
8.5050	$MnFe_2\sigma_4$	9.995	$FeCr_2S_4$
8.51	$MgRh_2\sigma_4$	10.011	$Lu_2Ti_2\sigma_7$
8.52	$Fe_2Ti\sigma_4$	10.02	$NaMgAl(F,\sigma H)_6 \cdot H_2\sigma$
8.52	$MnFe_2\sigma_4$	10.028	$Yb_2Ti_2\sigma_7$
8.52	$ZnRh_2\sigma_4$	10.050	$Tm_2Ti_2\sigma_7$
8.521	$Fe_2Ti\sigma_4$	10.065	$MnCr_2S_4$
8.53	$MgRh_2\sigma_4$	10.069	$Er_2Ti_2\sigma_7$
8.54	$ZnRh_2\sigma_4$	10.0762	$Er_2Ti_2\sigma_7$
8.540	$(Co,Sb)_3\sigma_4$	10.087	$Yb_2Ru_2\sigma_7$
8.55	$GdMg_2$	10.095	$Ho_2Ti_2\sigma_7$
8.551	$Fe_2Ti\sigma_4$	10.095	$Y_2Ti_2\sigma_7$
8.57	$MnRh\sigma_3$	10.096	$Tm_2Ru_2\sigma_7$
8.570	$Mg_2Th$	10.103	$Lu_2Ru_2\sigma_7$
8.575	$Mn_2V\sigma_4$	10.119	$Dy_2Ti_2\sigma_7$
8.584	$CdCr_2\sigma_4$	10.120	$Er_2Ru_2\sigma_7$
8.585	$Zn(Zn,Sb)_2\sigma_4$	10.144	$Y_2Ru_2\sigma_7$
8.589	$MnFe_2\sigma_4$	10.148	$Tb_2Ti_2\sigma_7$
8.59	$CdGa_2\sigma_4$	10.150	$Ho_2Ru_2\sigma_7$
8.597	$Mg_2Sn\sigma_4$	10.171	$Gd_2Ti_2\sigma_7$
8.60	$MnRh_2\sigma_4$	10.175	$Dy_2Ru_2\sigma_7$
8.61	$CdCr_2\sigma_4$	10.18	$Cd_2Sb_2\sigma_7$
8.613	$MnRh_2\sigma_4$	10.181	$Gd_2Ti_2\sigma_7$
8.622	$Co_2Sn\sigma_4$	10.19	$Ca_{33}Ge$
8.63	$Zn_2Sn\sigma_4$	10.192	$Eu_2Ti_2\sigma_7$
8.639	$Mg_2Sn\sigma_4$	10.20	$NaSb\sigma_3$
8.64	$Mn_3\sigma_4$	10.200	$Tb_2Ru_2\sigma_7$
8.644	$Co_2Sn\sigma_4$	10.206	$HgCr_2S_4$
8.667	$Zn_2Sn\sigma_4$	10.211	$CdCr_2S_4$
8.679	$Mn_2Ti\sigma_4$	10.211	$Sm_2Ti_2\sigma_7$
8.68	$CeMg_2$	10.215	$CdCr_2S_4$
8.69	$CdFe_2\sigma_4$	10.219	$Cd_2Re_2\sigma_7$
8.695	$Mn_2Ti\sigma_4$	10.230	$Gd_2Ru_2\sigma_7$
8.71	$CdFe_2\sigma_4$	10.24	$Tl_{1.31}Sb_4Sb_{16}\sigma_{48}$
8.73	$CeMg_2$	10.25	$Sb_{19}(\sigma,\sigma H)_{48} \cdot 12H_2\sigma$
8.76	$CdRh_2\sigma_4$	10.25	$CuSb_2(\sigma,\sigma H,H_2\sigma)_7$
8.781	$CdRh_2\sigma_4$	10.25	$AgSb\sigma_3$
8.79	$LaMg_2$	10.25	$Zr_3S_4$
8.83	$In_2Mg\sigma_4$	10.252	$Eu_2Ru_2\sigma_7$

Fd3m  $0_h^7$  No. 227 (continued)

## Inorganic (continued)

10.26	$Sb_2\sigma_4$	10.648	$Nd_2Hf_2\sigma_7$
10.26	$Sb_2\sigma_4 \cdot H_2\sigma$	10.648	$Nd_2Zr_2\sigma_7$
10.26	$TiZr_2S_4$	10.65	$Pb_2Yb\sigma_6$
10.280	$Sm_2Ru_2\sigma_7$	10.68	$NdPb_2Ta\sigma_6$
10.282	$(Ca,Na,Mn)_2Sb_2(\sigma, \sigma H, F)_7$	10.68	$[Pb_6Sb_4\sigma_{17}]$
10.285	$(Ca,Fe)_{11}(Nb,U,Ti,Ta)_{16}\sigma_{48}(\sigma H, F)_8$	10.69	$Pb_2YbNb\sigma_6$
10.288	$Ca_2Sb_2\sigma_7$	10.699	$Ce_2Zr_2\sigma_7$
10.29	$RbSb_5Sb_{16}\sigma_{48}$	10.70	$Pb_2SmTa\sigma_6$
10.290	$(Ca,Na,Fe)_2(Sb,Ti)_2(\sigma, \sigma H)_7$	10.70	$Pb_2YTa\sigma_6$
10.30	$SbSb_2\sigma_6\sigma H$	10.70	$Pb_2Sb_2\sigma_7$
10.30	$K_4Sb_4Sb_{16}\sigma_{48}$	10.702	$La_2Sn_2\sigma_7$
10.304	$Yb_2Sn_2\sigma_7$	10.704	$In_2S_3$
10.305	$Sb_2\sigma_5$	10.708	$MgIn_2S_4$
10.317	$(Ca,Na,Fe)_2Sb_2\sigma_6(\sigma H)$	10.715	$MnIn_2S_4$
10.32	$Ca_2Sb_2\sigma_7$	10.721	$CdCr_2Se_4$
10.331	$Nd_2Ru_2\sigma_7$	10.73	$Pb_2MnTa\sigma_6$
10.350	$Er_2Sn_2\sigma_7$	10.75	$Pb_2PrTa\sigma_6$
10.355	$Pr_2Ru_2\sigma_7$	10.757	$Mn_3Ni_2Si$
10.357	$CuCr_2Se_4$	10.771	$La_2Hf_2\sigma_7$
10.357	$FeNb_2\sigma_6$	10.78	$Ni_2SiV_3$
10.36	$HSb\sigma_3 \cdot 0.31H_2\sigma$	10.796	$CaIn_2S_4$
10.36	$NaSb\sigma_3$	10.807	$FeLu_2S_4$
10.362	$(Na,Ca)_2(Nb,Ti)_2(\sigma, F)_7$	10.81	$MoBe_2S_4$
10.367	$Li_7N_2I$	10.819	$CdIn_2S_4$
10.37	$Ca_2Ta_2\sigma_7$	10.833	$HgIn_2S_4$
10.37	$U_2Ta_2\sigma_7$	10.838	$FeYb_2S_4$
10.371	$Y_2Sn_2\sigma_7$	10.87	$Cu_2SnS_4$
10.372	$Cd_2Nb_2\sigma_7$	10.877	$CFe_3V_3$
10.376	$Cd_2Ta_2\sigma_7$	10.9	$ZnMn_2Se_4$
10.383	$(Ca,Ce,Na)_2(Nb,U,Ti)_2\sigma_6F$	10.921	$MnLu_2S_4$
10.39	$(Nb,Fe)_2(Ca,Ce,Na,K)_2\sigma_6(\sigma H, F, \sigma)$	10.94	$Cu_5FeS_4$
10.397	$[CaNaTa_2\sigma_7]$	10.949	$MgLu_2S_4$
10.397	$NaCaNb_2\sigma_6F$	10.949	$MnYb_2S_4$
10.4	$ZnMn_2S_4$	10.95	$Cu_5FeS_4$
10.404	$Pb_2Ti_2\sigma_6$	10.95	$CFe_6W_6$
10.42	$CaNaTa_2\sigma_6F$	10.957	$MgYb_2S_4$
10.42	$(Ca,Na,Sb)_2(Ta,Nb)_2\sigma_6(\sigma, \sigma H)$	10.973	$C(Co,Ni)_3(Cr,Mo)_3$
10.420	$Ca_2Ta_2\sigma_7$	11.0	$ZnMn_2Te_4$
10.426	$Y_2Zr_2\sigma_7$	11.051	$CuCr_2Te_4$
10.43	$Pb_2Sb_2\sigma_7$	11.06	$CFe_3W_3$
10.43	$(Ca,Na,Fe)_2(Nb,Ta,Ti)_2(\sigma, \sigma H, F)_7$	11.0680	$As_2\sigma_3$
10.443	$ZnCr_2Se_4$	11.090	$CCO_3W_3$
10.45	$KSb\sigma_3$	11.096	$CFe_2W_2$
10.46	$AgSb_2(\sigma, \sigma H, H_2\sigma)_7$	11.10	$Mn_3Ti_3\sigma$
10.460	$Gd_2Sn_2\sigma_7$	11.14	$Fe_3Ti_3\sigma$
10.47	$Pb_2Sb_2\sigma_7$	11.15	$Fe_3Ti_3\sigma$
10.474	$Eu_2Sn_2\sigma_7$	11.15	$Sb_2\sigma_3$
10.48	$BiTa_2\sigma_6F$	11.159	$Ni_2SiTa_3$
10.48	$Sn_2Ta_2\sigma_7$	11.16	$Co_3Ti_3\sigma$
10.485	$NiIn_2S_4$	11.178	$Nb_3Ni_2Si$
10.4973	$ZnCr_2Se_4$	11.18	$Ni_3Ti_3\sigma$
10.507	$Sm_2Sn_2\sigma_7$	11.196	$Co_2Nb_3Si$
10.51	$AlPb_2Ta\sigma_6$	11.24	$CuTi_2$
10.525	$FeSc_2S_4$	11.24	$Cu_3Ti_3\sigma$
10.53	$AlPb_2Nb\sigma_6$	11.262	$Fe_2Nb_3$
10.53	$Pb_2YbTa\sigma_6$	11.275	$Fe_2Ti_4\sigma$
10.532	$(Y,Ce,Th,Fe)_2Si_2\sigma_7$	11.278	$NiTi_2$
10.54	$CrPb_2Nb\sigma_6$	11.28	$Mn_2Ti_4\sigma$
10.551	$Pb_3Ta_4\sigma_{13}$	11.29	$Mn_2Ti_4\sigma$
10.56	$Pb_2MnNb\sigma_6$	11.295	$Co_2Ti_4\sigma$
10.56	$(Pb,Na,Ca)(Ta,Nb,Ti)_2\sigma_6(\sigma H)$	11.30	$Cr_3Ti_3\sigma$
10.562	$(Ba,Sr)(Nb,Ti)_2\sigma_6 \cdot H_2\sigma$	11.30	$CoTi_2$
10.563	$Sn_2Ta_2\sigma_7$	11.30	$Ni_2Ti_4\sigma$
10.573	$Nd_2Sn_2\sigma_7$	11.31	$Fe_2Ti_4\sigma$
10.580	$CoIn_2S_4$	11.3193	$NiTi_2$
10.59	$(Na,K,Mg,Ca,Ba,RE,Th,Pb)_{0.614}(Ti,Nb,Ta)_{2.00}(H_2\sigma)_{1.64}\sigma_{5.52}$	11.32	$Co_2Ti_4\sigma$
10.6	$Cu_2MoS_4$	11.3279	$Ni_2Ti_4\sigma$
10.604	$Pr_2Sn_2\sigma_7$	11.37	$Ni_2Ti_4\sigma$
10.619	$FeIn_2S_4$	11.4353	$Cu_2Ti_4\sigma$
10.62	$CrNi_xSi_y$	11.44	$Cu_2Ti_4\sigma$
10.62	$FeIn_2S_4$	11.47	$Cu_2Ti_4\sigma$
10.623	$MnSc_2S_4$	11.49	$CCr_3Nb_3$
10.627	$MgSc_2S_4$	11.51	$CCO_2(Ti,Ta)_4$
		11.549	$Nb_3Zn_3\sigma_{0.4}$



Fd3m  $O_h^7$  No. 227 (continued)

## Inorganic (continued)

11.561	Be <sub>2</sub> Re	14.53	Al <sub>18</sub> Cr <sub>2</sub> Mg <sub>3</sub>
11.618	CCo <sub>3</sub> Ta <sub>3</sub>	14.586	Al <sub>11</sub> V
11.631	Be <sub>2</sub> W	14.62	Na <sub>x</sub> Si <sub>136</sub>
11.633	CCo <sub>3</sub> Nb <sub>3</sub>	16.2	Sr <sub>4</sub> (Ir <sub>0.75</sub> Pt <sub>0.25</sub> ) <sub>6</sub>
11.634	Be <sub>2</sub> Mo	23.0	Ni <sub>2</sub> SiMo <sub>12</sub> <sup>θ</sup> <sub>40</sub> •31H <sub>2</sub> <sup>θ</sup>
11.698	CNb <sub>3</sub> Ni <sub>3</sub>	23.09	Mg <sub>2</sub> SiMo <sub>12</sub> <sup>θ</sup> <sub>40</sub> •31H <sub>2</sub> <sup>θ</sup>
12.120	NiSc <sub>2</sub>	23.1	H <sub>3</sub> PMo <sub>12</sub> <sup>θ</sup> <sub>40</sub> •30H <sub>2</sub> <sup>θ</sup>
12.3255	Hf <sub>2</sub> Rh	23.1	SmPMo <sub>12</sub> <sup>θ</sup> <sub>40</sub> •30H <sub>2</sub> <sup>θ</sup>
12.352	Hf <sub>2</sub> Ir	23.10	Ba <sub>3</sub> (Pθ <sub>4</sub> Mo <sub>12</sub> <sup>θ</sup> <sub>36</sub> ) <sub>2</sub> •58H <sub>2</sub> <sup>θ</sup>
12.3605	Hf <sub>2</sub> Pd	23.10	Sr <sub>3</sub> (Pθ <sub>4</sub> Mo <sub>12</sub> <sup>θ</sup> <sub>36</sub> ) <sub>2</sub> •58H <sub>2</sub> <sup>θ</sup>
12.427	PdSc <sub>2</sub>	23.10	Zn <sub>3</sub> (Pθ <sub>4</sub> Mo <sub>12</sub> <sup>θ</sup> <sub>36</sub> ) <sub>2</sub> •58H <sub>2</sub> <sup>θ</sup>
12.461	Hf <sub>2</sub> Pt	23.11	Ca <sub>3</sub> (Pθ <sub>4</sub> Mo <sub>12</sub> <sup>θ</sup> <sub>36</sub> ) <sub>2</sub> •58H <sub>2</sub> <sup>θ</sup>
12.467	RhZr <sub>2</sub>	23.11	Co <sub>3</sub> (Pθ <sub>4</sub> Mo <sub>12</sub> <sup>θ</sup> <sub>36</sub> ) <sub>2</sub> •58H <sub>2</sub> <sup>θ</sup>
12.47	IrZr <sub>2</sub>	23.11	Mg <sub>3</sub> (Pθ <sub>4</sub> Mo <sub>12</sub> <sup>θ</sup> <sub>36</sub> ) <sub>2</sub> •58H <sub>2</sub> <sup>θ</sup>
12.529	K <sub>2</sub> Zn(CN) <sub>4</sub>	23.11	Mn <sub>3</sub> (Pθ <sub>4</sub> Mo <sub>12</sub> <sup>θ</sup> <sub>36</sub> ) <sub>2</sub> •58H <sub>2</sub> <sup>θ</sup>
12.79	HgK <sub>2</sub> (CN) <sub>4</sub>	23.11	Ni <sub>3</sub> (Pθ <sub>4</sub> Mo <sub>12</sub> <sup>θ</sup> <sub>36</sub> ) <sub>2</sub> •58H <sub>2</sub> <sup>θ</sup>
12.87	CdK <sub>2</sub> (CN) <sub>4</sub>	23.13	Cd <sub>3</sub> (Pθ <sub>4</sub> Mo <sub>12</sub> <sup>θ</sup> <sub>36</sub> ) <sub>2</sub> •58H <sub>2</sub> <sup>θ</sup>
13.86	BaCd <sub>2</sub> Cl <sub>6</sub>	23.15	FeHSiW <sub>12</sub> <sup>θ</sup> <sub>40</sub> •30H <sub>2</sub> <sup>θ</sup>
13.90	BaCd <sub>2</sub> Cl <sub>6</sub> •5H <sub>2</sub> <sup>θ</sup>	23.15	NdPMo <sub>12</sub> <sup>θ</sup> <sub>40</sub> •30H <sub>2</sub> <sup>θ</sup>
14.075	HfZr <sub>2</sub>	23.3	Be <sub>2</sub> SiW <sub>12</sub> <sup>θ</sup> <sub>40</sub> •31H <sub>2</sub> <sup>θ</sup>
14.08	Na <sub>3</sub> MgCl(Cθ <sub>3</sub> ) <sub>2</sub>	23.328	H <sub>3</sub> PW <sub>12</sub> <sup>θ</sup> <sub>40</sub> •29H <sub>2</sub> <sup>θ</sup>
14.101	Zn <sub>2</sub> Zr	24.60	Na <sub>2</sub> Ca(AlSi <sub>2</sub> <sup>θ</sup> <sub>6</sub> ) <sub>4</sub> •16H <sub>2</sub> <sup>θ</sup>
14.20	MgNa <sub>3</sub> Br(Cθ <sub>3</sub> ) <sub>2</sub>	28.239	Al <sub>3.22</sub> Mg <sub>2</sub>
14.492	Al <sub>10</sub> V	30.56	Cd <sub>2</sub> Na

## Organic

3.56	C	11.633	Co <sub>3</sub> Nb <sub>3</sub> C
10.877	Fe <sub>3</sub> V <sub>3</sub> C	11.698	Nb <sub>3</sub> Ni <sub>3</sub> C
10.95	Fe <sub>6</sub> W <sub>6</sub> C	12.529	K <sub>2</sub> Zn(CN) <sub>4</sub>
10.973	C(Cr,Mo) <sub>3</sub> (Co,Ni) <sub>3</sub>	12.79	HgK <sub>2</sub> (CN) <sub>4</sub>
11.06	Fe <sub>3</sub> W <sub>3</sub> C	12.87	CdK <sub>2</sub> (CN) <sub>4</sub>
11.090	Co <sub>3</sub> W <sub>3</sub> C	14.08	Na <sub>3</sub> MgCl(Cθ <sub>3</sub> ) <sub>2</sub>
11.096	Fe <sub>2</sub> W <sub>2</sub> C	14.20	Na <sub>3</sub> MgBr(Cθ <sub>3</sub> ) <sub>2</sub>
11.271	C(CH <sub>3</sub> ) <sub>4</sub>	16.43	Zn <sub>4</sub> <sup>θ</sup> (CH <sub>3</sub> Cθ <sup>θ</sup> ) <sub>6</sub>
11.49	Cr <sub>3</sub> Nb <sub>3</sub> C	17.31	8C <sub>4</sub> H <sub>8</sub> <sup>θ</sup> •7.33H <sub>2</sub> S•136H <sub>2</sub> <sup>θ</sup>
11.51	Co <sub>2</sub> (Ti,Ta) <sub>4</sub> C	18.24	(C <sub>2</sub> H <sub>5</sub> •Cθ <sup>θ</sup> ) <sub>6</sub> BaCa <sub>2</sub>
11.618	Co <sub>3</sub> Ta <sub>3</sub> C		

 $\frac{4}{m} \frac{3}{m} \frac{2}{m}$ Fd3c  $O_h^8$  No. 228Inorganic - 2  
Organic - 0

## Inorganic

15.51	Te(Cθ) <sub>6</sub>	27.92	Na <sub>5</sub> (Pθ <sub>4</sub> ) <sub>2</sub> F•19H <sub>2</sub> <sup>θ</sup>
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## Organic

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 $\frac{4}{m} \frac{3}{m} \frac{2}{m}$ Im3m  $O_h^9$  No. 229Inorganic - 80  
Organic - 3

## Inorganic

2.5515	Be	3.30656	Nb
2.859	(Fe,B)	3.3163	Ta <sup>θ</sup> <sub>x</sub>
2.866	(Fe,Ni,Co)	3.33	Ti
2.86645	Fe	3.36	Ta-B
2.88495	Cr	3.44	U
2.902	(Fe,Al)	3.5090	Li
2.94	Fe	3.62	Zr
2.975	FeTi	3.6361	Pu
2.986	NiTi	3.8734	S
2.994	CoTi	3.882	Tl
3.015	GaV	4.02	Al
3.0399	V	4.12	Ce
3.060	Mn-Zn	4.26	La
3.1472	Mo	4.2906	Na
3.16529	W	4.477	Ca
3.25	Ag <sub>3</sub> Al	4.582	Eu
3.282	Ti	4.85	Sr
3.3058	Ta	4.87	Sr

Im3m  $O_h^9$  No. 229 (continued)

## Inorganic (continued)

4.870	Ag <sub>2</sub> S	8.850	Ni <sub>6</sub> Si <sub>2</sub> Sm <sub>3</sub>
4.993	Ag <sub>2</sub> Se	8.858	Ce <sub>3</sub> Ni <sub>6</sub> Si <sub>2</sub>
5.025	Ba	8.907	Nd <sub>3</sub> Ni <sub>6</sub> Si <sub>2</sub>
5.044	AgI	8.913	Eu <sub>3</sub> Ni <sub>6</sub> Si <sub>2</sub>
5.344	K	8.95	Fe <sub>3</sub> Zn <sub>10</sub>
5.63	Rb	8.976	Ni <sub>6</sub> Pr <sub>3</sub> Si <sub>2</sub>
6.091	Ca	9.10	Ca(NH <sub>3</sub> ) <sub>6</sub>
7.678	HPF <sub>6</sub> •6H <sub>2</sub> O	9.351	Ru <sub>3</sub> Sn <sub>7</sub>
7.87	HNbF <sub>6</sub> •6H <sub>2</sub> O	9.360	Ir <sub>3</sub> Sn <sub>7</sub>
7.88	HTaF <sub>6</sub> •6H <sub>2</sub> O	9.364	Ru <sub>3</sub> Sn <sub>7</sub>
8.031	Hg <sub>6</sub> Cl <sub>4</sub> O	9.416	In <sub>7</sub> Pt <sub>3</sub>
8.190	Nb <sub>6</sub> F <sub>15</sub>	9.55	Sr(NH <sub>3</sub> ) <sub>6</sub>
8.659	Lu <sub>3</sub> Ni <sub>6</sub> Si <sub>2</sub>	9.5688	Mo <sub>3</sub> Sb <sub>7</sub>
8.662	Ni <sub>6</sub> Si <sub>2</sub> Yb <sub>3</sub>	9.5713	Mo <sub>3</sub> Sb <sub>7</sub>
8.696	Ni <sub>6</sub> Si <sub>2</sub> Tm <sub>3</sub>	9.609	Re <sub>24</sub> Ti <sub>5</sub>
8.714	As <sub>7</sub> Re <sub>3</sub>	9.76	FeTi <sub>x</sub>
8.725	Er <sub>3</sub> Ni <sub>6</sub> Si <sub>2</sub>	9.95	Ba(NH <sub>3</sub> ) <sub>6</sub>
8.735	Ge <sub>7</sub> Ir <sub>3</sub>	10.0	Na <sub>6</sub> (Si <sub>10</sub> Al <sub>6</sub> )O <sub>32</sub> •12H <sub>2</sub> O
8.742	Ho <sub>3</sub> Ni <sub>6</sub> Si <sub>2</sub>	10.1	Ag <sub>2</sub> Hg <sub>3</sub>
8.763	Dy <sub>3</sub> Ni <sub>6</sub> Si <sub>2</sub>	10.11	Ag <sub>3</sub> Hg <sub>4</sub>
8.801	Ni <sub>6</sub> Si <sub>2</sub> Tb <sub>3</sub>	11.61	Sb <sub>2</sub> Tl <sub>7</sub>
8.838	Gd <sub>3</sub> Ni <sub>6</sub> Si <sub>2</sub>	22.85	Co(NH <sub>3</sub> ) <sub>6</sub> (ClO <sub>4</sub> ) <sub>3</sub>

## Organic

7.51	C <sub>2</sub> Cl <sub>6</sub>	13.25	NH <sub>4</sub> [Cr(NCS) <sub>4</sub> (NH <sub>3</sub> ) <sub>2</sub> ]•2/3H <sub>2</sub> O
8.17	C(SCH <sub>3</sub> ) <sub>4</sub>		

 $\frac{4}{m} \frac{3}{m} \frac{2}{m}$ Ia3d  $O_h^{10}$  No. 230Inorganic - 132  
Organic - 0

## Inorganic

8.565	Cd <sub>2x</sub> Bi <sub>1-2x</sub> O <sub>3-x</sub>	12.11	Gd <sub>3</sub> Al <sub>2</sub> (AlO <sub>4</sub> ) <sub>3</sub>
11.455	Mg <sub>3</sub> Al <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.12	Ca <sub>3</sub> Al <sub>2</sub> Ge <sub>3</sub> O <sub>12</sub>
11.520	Al <sub>2</sub> Fe <sub>3</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.121	Al <sub>2</sub> Na <sub>3</sub> (LiF <sub>4</sub> ) <sub>3</sub>
11.526	[Fe <sub>3</sub> Al <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub> ]	12.125	Mn <sub>3</sub> V <sub>2</sub> Ge <sub>3</sub> O <sub>12</sub>
11.533	Al <sub>2</sub> (Mg, Fe) <sub>3</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.128	Ca <sub>3</sub> Fe <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>
11.61	Al <sub>2</sub> Mn <sub>3</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.16	Ca <sub>3</sub> Al <sub>2</sub> Si <sub>2</sub> O <sub>10</sub> •2H <sub>2</sub> O
11.613	(Mn, Fe, Ca, Mg) <sub>3</sub> (Al, Fe) <sub>2</sub> [(Si, Al)O <sub>4</sub> ] <sub>3</sub>	12.168	Ca <sub>3</sub> Fe <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>
11.692	(Al, Fe) <sub>2</sub> (Fe, Ca) <sub>3</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.188	Lu <sub>3</sub> Ga <sub>2</sub> (GaO <sub>4</sub> ) <sub>3</sub>
11.697	(Mn, Ca) <sub>3</sub> (Al, Fe) <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.204	Yb <sub>3</sub> Ga <sub>2</sub> (GaO <sub>4</sub> ) <sub>3</sub>
11.819	Fe <sub>2</sub> Mn <sub>3</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.213	Cd <sub>3</sub> Cr <sub>2</sub> (GeO <sub>4</sub> ) <sub>3</sub>
11.841	Ca <sub>3</sub> (Al, Fe) <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.25	Er <sub>3</sub> Ga <sub>2</sub> (GaO <sub>4</sub> ) <sub>3</sub>
11.855	[Ca <sub>3</sub> Cr <sub>2</sub> Si <sub>3</sub> O <sub>12</sub> ]	12.27	Cd <sub>3</sub> Mn <sub>2</sub> Ge <sub>3</sub> O <sub>12</sub>
11.8550	Al <sub>2</sub> Ca <sub>3</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.27	Ca <sub>3</sub> Sc <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>
11.864	Al <sub>2</sub> Ca <sub>3</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.275	Ca <sub>3</sub> Cr <sub>2</sub> (GeO <sub>4</sub> ) <sub>3</sub>
11.895	Mn <sub>3</sub> Al <sub>2</sub> (GeO <sub>4</sub> ) <sub>3</sub>	12.277	Lu <sub>3</sub> Fe <sub>2</sub> (FeO <sub>4</sub> ) <sub>3</sub>
11.906	Lu <sub>3</sub> Al <sub>2</sub> (AlO <sub>4</sub> ) <sub>3</sub>	12.285	Cd <sub>3</sub> Rh <sub>2</sub> Ge <sub>3</sub> O <sub>12</sub>
11.91	(Al, Fe) <sub>2</sub> Ca <sub>3</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.29	Cd <sub>3</sub> V <sub>2</sub> Ge <sub>3</sub> O <sub>12</sub>
11.931	Ca <sub>3</sub> (Al, Fe) <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.291	Yb <sub>3</sub> Fe <sub>2</sub> (FeO <sub>4</sub> ) <sub>3</sub>
11.931	Yb <sub>3</sub> Al <sub>2</sub> (AlO <sub>4</sub> ) <sub>3</sub>	12.30	Y <sub>3</sub> Ge <sub>2</sub> (GaO <sub>4</sub> ) <sub>3</sub>
11.956	(Fe, Al) <sub>2</sub> (Ca, Fe, Mg, Mn) <sub>3</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.300	CoY <sub>2</sub> Co <sub>2</sub> Ge <sub>3</sub> O <sub>12</sub>
11.957	Tm <sub>3</sub> Al <sub>2</sub> Al <sub>3</sub> O <sub>12</sub>	12.31	MgGd <sub>2</sub> Mg <sub>2</sub> Ge <sub>3</sub> O <sub>12</sub>
11.974	Ca <sub>3</sub> Cr <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.312	Ca <sub>3</sub> Fe <sub>2</sub> (GeO <sub>4</sub> ) <sub>3</sub>
11.98	Er <sub>3</sub> Al <sub>2</sub> (AlO <sub>4</sub> ) <sub>3</sub>	12.32	Ca <sub>3</sub> TiNiGe <sub>3</sub> O <sub>12</sub>
12.01	Y <sub>3</sub> Al <sub>2</sub> (AlO <sub>4</sub> ) <sub>3</sub>	12.32	Dy <sub>3</sub> Ga <sub>2</sub> (GaO <sub>4</sub> ) <sub>3</sub>
12.011	Ho <sub>3</sub> Al <sub>2</sub> Al <sub>3</sub> O <sub>12</sub>	12.325	Ca <sub>3</sub> Mn <sub>2</sub> Ge <sub>3</sub> O <sub>12</sub>
12.02	Y <sub>3</sub> Al <sub>2</sub> (AlO <sub>4</sub> ) <sub>3</sub>	12.325	Tm <sub>3</sub> Fe <sub>2</sub> (FeO <sub>4</sub> ) <sub>3</sub>
12.02	Ca <sub>3</sub> (Al <sub>0.80</sub> Fe <sub>0.20</sub> ) <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.349	Er <sub>3</sub> Fe <sub>2</sub> (FeO <sub>4</sub> ) <sub>3</sub>
12.027	Cr <sub>2</sub> Mn <sub>3</sub> (GeO <sub>4</sub> ) <sub>3</sub>	12.35	Ca <sub>3</sub> In <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>
12.03	Cd <sub>3</sub> V <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>	12.35	Ca <sub>3</sub> Rh <sub>2</sub> Ge <sub>3</sub> O <sub>12</sub>
12.03	Li <sub>3</sub> AlF <sub>6</sub>	12.35	Ca <sub>3</sub> TiCoGe <sub>3</sub> O <sub>12</sub>
12.054	Ca <sub>3</sub> Fe <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.35	Ca <sub>3</sub> TiMgGe <sub>3</sub> O <sub>12</sub>
12.06	Dy <sub>3</sub> Al <sub>2</sub> (AlO <sub>4</sub> ) <sub>3</sub>	12.35	Ca <sub>3</sub> V <sub>2</sub> Ge <sub>3</sub> O <sub>12</sub>
12.070	Ca <sub>3</sub> V <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>	12.37	(Ca, Na) <sub>3</sub> (Mg, Mn) <sub>2</sub> (AsO <sub>4</sub> ) <sub>3</sub>
12.074	Tb <sub>3</sub> Al <sub>2</sub> Al <sub>3</sub> O <sub>12</sub>	12.376	Fe <sub>2</sub> Y <sub>3</sub> (FeO <sub>4</sub> ) <sub>3</sub>
12.079	(Ca, Mg, Mn) <sub>3</sub> (Fe, Al) <sub>2</sub> (Si, Sn) <sub>3</sub> O <sub>12</sub>	12.380	Ho <sub>3</sub> Fe <sub>2</sub> (FeO <sub>4</sub> ) <sub>3</sub>
12.080	(Ca, Mg) <sub>3</sub> (Fe, Al) <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.380	Y <sub>3</sub> Fe <sub>2</sub> Fe <sub>3</sub> O <sub>12</sub>
12.084	Ca <sub>3</sub> Fe <sub>2</sub> (SiO <sub>4</sub> ) <sub>3</sub>	12.39	Gd <sub>3</sub> Ga <sub>2</sub> (GaO <sub>4</sub> ) <sub>3</sub>
12.087	Fe <sub>2</sub> Mn <sub>3</sub> (GeO <sub>4</sub> ) <sub>3</sub>	12.392	MnY <sub>2</sub> Mn <sub>2</sub> Ge <sub>3</sub> O <sub>12</sub>
12.09	Ca <sub>3</sub> V <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>	12.395	MgGd <sub>2</sub> Mn <sub>2</sub> Ge <sub>3</sub> O <sub>12</sub>

Ia3d  $O_h^{10}$  No. 230 (continued)

## Inorganic (continued)

12.401	$\text{Eu}_3\text{Ga}_2(\text{Ga}\theta_4)_3$	12.504	$\text{Ca}_3\text{Sc}_2\text{Ge}_3\theta_{12}$
12.401	$\text{Gd}_3\text{Ni}_2\text{GaGe}_2\theta_{12}$	12.514	$\text{Ca}_3\text{ZrMgGe}_3\theta_{12}$
12.402	$\text{CoGd}_2\text{Co}_2\text{Ge}_3\theta_{12}$	12.515	$\text{Cd}_3\text{In}_2\text{Ge}_3\theta_{12}$
12.413	$\text{NiGd}_2\text{Mn}_2\text{Ge}_3\theta_{12}$	12.518	$\text{Eu}_3\text{Fe}_2(\text{Fe}\theta_4)_3$
12.414	$\text{Dy}_3\text{Fe}_2(\text{Fe}\theta_4)_3$	12.524	$\text{Sm}_3\text{Fe}_2(\text{Fe}\theta_4)_3$
12.42	$\text{Sm}_3\text{Ga}_2(\text{Ga}\theta_4)_3$	12.54	$\text{Ca}_3\text{ZrCoGe}_3\theta_{12}$
12.425	$\text{Gd}_3\text{Mg}_2\text{GaGe}_2\theta_{12}$	12.540	$\text{Sm}_3\text{Fe}_2(\text{Fe}\theta_4)_3$
12.427	$\text{ZnGd}_2\text{Mn}_2\text{Ge}_3\theta_{12}$	12.550	$\text{Gd}_3\text{Mn}_2\text{GaGe}_2\theta_{12}$
12.436	$\text{Tb}_3\text{Fe}_2(\text{Fe}\theta_4)_3$	12.555	$\text{CaGd}_2\text{Mn}_2\text{Ge}_3\theta_{12}$
12.437	$\text{CoGd}_2\text{Mn}_2\text{Ge}_3\theta_{12}$	12.57	$\text{Pr}_3\text{Ga}_2(\text{Ga}\theta_4)_3$
12.44	$\text{Fe}_5\text{Gd}_3\theta_{12}$	12.573	$\text{Ca}_3\text{Al}_2(\theta\text{H})_{12}$
12.446	$\text{Gd}_3\text{Co}_2\text{GaGe}_2\theta_{12}$	12.62	$\text{Ca}_3\text{In}_2\text{Ge}_3\theta_{12}$
12.447	$\text{Tb}_3\text{Fe}_2(\text{Fe}\theta_4)_3$	12.76	$\text{Ca}_3\text{Fe}_2(\theta\text{H})_{12}$
12.46	$\text{Ca}_3(\text{Zr},\text{Ti},\text{Mg},\text{Fe},\text{Nb})_2(\text{Al},\text{Fe},\text{Si})_3\theta_{12}$	13.05	$\text{Sr}_3\text{Al}_2(\theta\text{H})_{12}$
12.464	$\text{Gd}_3\text{Zn}_2\text{GaGe}_2\theta_{12}$	13.392	$\text{Hg}_3\text{Te}\theta_6$
12.47	$\text{Ca}_3\text{SnCoGe}_3\theta_{12}$	13.43	$\text{KAlSi}_2\theta_6$
12.470	$\text{Gd}_3\text{Fe}_2\text{Fe}_3\theta_{12}$	13.66	$\text{CsFeSi}_2\theta_6$
12.473	$\text{CdGd}_2\text{Mn}_2\text{Ge}_3\theta_{12}$	13.673	$\text{CsAlSi}_2\theta_6 \cdot 0.5\text{H}_2\theta$
12.475	$\text{CaY}_2\text{Mn}_2\text{Ge}_3\theta_{12}$	13.712	$\text{NaAlSi}_2\theta_6 \cdot \text{H}_2\theta$
12.475	$\text{CuGd}_2\text{Mn}_2\text{Ge}_3\theta_{12}$	13.73	$\text{NaAlSi}_2\theta_6 \cdot \text{H}_2\theta$
12.479	$\text{Gd}_3\text{Fe}_2(\text{Fe}\theta_4)_3$	14.9274	$\text{Bi}_4\text{Rh}$
12.482	$\text{MnGd}_2\text{Mn}_2\text{Ge}_3\theta_{12}$	20.286	$(\text{Ta}_6\text{Cl}_{12})\text{Cl}_3$
12.49	$(\text{Ca},\text{Na})_3(\text{Mn},\text{Mg})_2(\text{As}\theta_4)_3$	20.53	$\text{Rb}_4\text{PdAu}_2\text{Cl}_{12}$
12.49	$\text{Mn}_3\text{NbZnFeGe}_2\theta_{12}$	20.55	$\text{Rb}_4\text{CuAu}_2\text{Cl}_{12}$
12.490	$(\text{Nd}_{0.5}\text{Y}_{0.5})_3\text{Fe}_2(\text{Fe}\theta_4)_3$	20.91	$\text{Cs}_2\text{PdAu}_2\text{Cl}_{12}$
12.50	$\text{Ca}_3\text{ZrNiGe}_3\theta_{12}$	20.94	$\text{Cs}_4\text{CuAu}_2\text{Cl}_{12}$
12.50	$\text{Nd}_3\text{Ga}_2(\text{Ga}\theta_4)_3$	21.290	$(\text{Ta}_6\text{Br}_{12})\text{Br}_3$

## Organic

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