NIST Standard Reference Database 3

NIST Crystal Data

CD-ROM Guide

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INTRODUCTION

The NIST Crystallographic Data Center collects, evaluates and disseminates data on solid-state materials. NIST Crystal Data is a comprehensive database with chemical, physical and crystallographic information on all classes of well-characterized substances. These materials fall into the following categories: inorganics, organics, organometallics, metals, intermetallics and minerals. For each entry, data types include lattice parameters, crystal system, space group, chemical name, chemical formula, literature reference, among others.

NIST Crystal Data is being distributed in a multi-file format for ease of incorporation in other database management systems and processing by independent software routines. The following documentation describes the content and format of each of the ASCII data files. These files should be processed using column-specified fields, not blank-delimited fields, since there may be internal codes in fields not specified in this documentation. Most of the files contain one line per entry. Note that there may be more than one formula, name, literature reference, or comment per entry; these are unique and separate items and will be qualified by the addition of a sequence number.

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au-p1 : Authors cell, experimental conditions

Columns	Field
2-7	ID
11-19	a (Original Data) in Angstroms (1 A=10^{-10} m)
20-28	b
29-37	c
38-45	α (Original Data) in degrees
46-53	β
54-61	γ
62	Editorial code for cell Blank = cell given by author; normal temperature and pressure E = cell inserted by Crystal Data editor C = cell is Crystal Data cell (not necessarily the author's original cell) T = cell data is at high or low temperature P = cell data is at high pressure (may also be at high or low temperature)
75	Radiation of study Blank = not specified X = x-ray N = neutron E = electron G = gamma
77	Source of unit cell data Blank = not specified S = single crystal P = powder diffraction R = Rietveld or profile fit analysis
79	Structure code N = no information about structure is given L = limited structure information is given (partial structure determined or assigned by type) T = total structure determined (excluding H atoms)
82	Internal update code

84	Crystal system code A = anorthic (triclinic) M = monoclinic O = orthorhombic R = rhombohedral (hexagonal or rhombohedral axes) T = tetragonal H = hexagonal C = cubic

au-p2 : Authors space group, Z, and density

Columns	Field
2-7	ID
11-18	Author's space group, aspect in Laue class, or cell centering (left-justified)
19	Editorial code for space group Blank = space group given by author E = space group inserted by Crystal Data editor T = space group orientation corresponds to that of the Crystal Data cell (rare; orthorhombic only)
21	Aspect code Blank = Normal * = aspect number has been assigned
22-24	Space group or aspect number
25	Orientation code for space group or aspect
30-35	Z (number of formula units per unit cell)
36	Editorial code for Z Blank = Z given by author E = Z has been inserted by the Crystal Data editor G = Z has been guessed
40-45	Dm (author's measure density) in Mg/m^3(g/cm^3)
48-53	Dx (author's calculate density) in Mg/m^3
71-79	Input cell volume
82	Internal update code

au-p3 : Authors standard deviations for cell parameters

Columns	Field
2-7	ID
11-19	σ (a)
20-28	σ (b)
29-37	σ (c)
38-45	σ (α)
46-53	σ (β)
54-61	σ (γ)
63-66	Average error in axial lengths in parts per 10^5
67	Editorial code for average error Blank = standard deviations reported by the authors E = editorial errors assigned
69-79	Quality index code for cell
82	Internal update code

cd-p1 : *Crystal Data cell, axial ratios*

Columns	Field
2-7	ID
11-18	a (Crystal Data cell) in Angstroms
19-26	b
27-34	c
35-41	α (Crystal Data cell) in degrees
42-48	β
49-55	γ
56-64	First determinative ratio The first determinative ratio is a/b for the anorthic, monoclinic, and orthorhombic crystal systems; c/a for the tetragonal, hexagonal and rhombohedral (H axes) systems; and a for the cubic system.
65-72	Second determinative ratio The second determinative ratio is c/b for the anorthic, monoclinic and orthorhombic systems; it is blank for the tetragonal, hexagonal, rhombohedral and cubic systems.
82	Internal update code

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cd-p2 : Crystal Data space group, Z, and density

Columns	Field
2-7	ID
11-18	Crystal Data space group, aspect, or centering (left-justified)
19	Editorial code for space group Blank = normal E = original space group is editorial
21	Aspect code Blank = normal * = aspect number assigned
22-24	Space group number or aspect number
25	Orientation code for space group or aspect
30-35	Z for Crystal Data cell
36	Editorial code for Crystal Data Z Blank = normal E = original Z is editorial G = original Z is guessed
40-44	Density approximated by atomic volumes in Mg/m^3
45	A (editorial code for approximate density)
48-53	Dx (program calculated density)
54	Editorial code for Dx Blank = normal G = Dx is questionable due to guessed or missing Z, or to approximation of empirical formula
61-68	Molecular or formula weight
69	Editorial code for molecular weight Blank = normal G = molecular weight is questionable due to approximation of empirical formula
71-79	Volume of Crystal Data cell
82	Internal update code

cd-trans : Matrix for authors cell → Crystal Data cell

Columns	Field
2-7	ID
11-14	Determinant of transformation matrix
15	:
17-34	First row of transformation matrix
35	/
36-53	Second row of transformation matrix
54	/
55-72	Third row of transformation matrix
82	Internal update code

cpd-flag : Material, class and registration indicators

Columns	Field
2-7	ID
11	I for inorganic material (blank if not)
12	O for organic material (blank if not)
13	M for mineral (blank if not)
14	A for alloy, metal, intermetallic material (blank if not)
35-62	Chemical class indicators (organic) or mineral group codes (inorganic)
64-74	Chemical Abstracts Service (CAS) registry number
82	Internal update code

cpd-name : *Compound name*

Columns	Field
2-7	ID
9	Sequence number
11	Index code

Blank = Crystal Data index name
M = mineral name
N = chemical name for a mineral
C = common or trivial name
D = name to be omitted from index

13-end	Compound name

ele-subs : *Element subscript*

Columns	Field
2-7	ID
10-11	Element count
13-17	Number of atoms for element symbol #1
19-23	Number of atoms for element symbol #2
25-29	Number of atoms for element symbol #3
.	.
.	.
End	Number of atoms for element symbol #=element count

ele-symb : *Element symbol*

Columns	Field
2-7	ID
10-11	Element count
13-15	Element symbol #1
17-19	Element symbol #2
21-23	Element symbol #3
.	.
.	.
End	Element symbol #=element count

(Note: the symbols Ln or TR may be used for unspecified rare earth elements.)

for-chem : Chemical formula

Columns	Field
2-7	ID
9	Sequence number
11	Formula approximation code Blank = normal G = editor has simplified formula or composition is approximate (e.g. for minerals)
13	Formula editorial code Blank = normal A = formula is absent D = omit from index X = pseudo-empirical formula index (organic only) P = permuted formula index (organic only)
15-end	Chemical formula

(Note: the symbols Ln or TR may be used for unspecified rare earth elements.)

for-emp : *Empirical formula*

Columns	Field
2-7	ID
9	Approximation code Blank = normal G = formula is approximate or simplified
11	Editorial code Blank = empirical formula was generated from the chemical formula E = empirical formula inserted by editor
13-end	Empirical formula

lit-refs : *Literature reference*

Columns	Field
2-7	ID
9-10	Sequence number
12-13	Code for reference Blank = primary journal reference CD = reference from Volume 1 or 2 of Crystal Data Determinative Tables
15-20	CODEN
22-25	Volume number
27-31	Page number
33-36	Year
38-end	Authors

rd-p1 : Reduced cell, metric symmetry

Columns	Field
2-7	ID
11-18	a (reduced cell) in Angstroms
19-26	b
27-34	c
35-41	α (reduced cell) in degrees
42-48	β
49-55	γ
56-64	Volume (reduced cell)
76-77	Reduced form number
78	Metric symmetry code Blank = normal X = metric symmetry exceeds crystal symmetry
82	Internal update code

str-type : Structure type

Columns	Field
2-7	ID
11-19	Pearson symbol for alloys, metals, and intermetallics
20	Editorial code for Pearson symbol Blank = normal (generated from empirical formula and Z) E = Pearson symbol inserted by Crystal Data editor
28-77	Structure type (formula, name, or Strukturbericht designation)
82	Internal update code

comments : *Comments*

Columns	Field
2-7	ID
9-10	Sequence number
12-13	Comment code Blank = General comment SM = Sample source or locality PR = Sample preparation ST = Structure CL = Color AN = Analysis OP = Optical data PM = Polymorphism AD = Additional pattern MP = Melting point CR = Cross-reference (added at production time) LN = Additional diffraction line(s) AX = Axial ratio data UC = Unit cell data TM = Temperature of data collected PD = Powder data HK = Footnotes for hkl and superlattice d-spacings OO = Reason 'O' quality was assigned (PDF code) FN = Footnote for d-spacings DB = Deleted by or rejected by

	AT = Atomic positions
	TH = Thermal parameters
	FF = Scattering factors
	SC = Scale factors
15-end	Comment

process1 : *Update or revision*

Columns	Field
2-7	ID
11-18	Revision date (year/month/day)
20-22	Initials (revision by)
24-78	Information on items revised or corrected
82	Internal update code

process2 : *Processing history*

Columns	Field
2-7	ID
11-18	Entry date (inorganic) or accession date (organic) in the form year/month/day
21-28	Keyboarding date (inorganic) or modification date (organic) (year/month/day)
30-32	Initials of keyboarder
34-41	Processing date (year/month/day)
42-44	Number of warnings
45-47	Number of errors
49-50	Processing program revision number
52-59	Revision date (year/month/day)
61-67	PDF number (reference to the Powder Diffraction File of the International Centre for Diffraction Data)
69-76	Alternate reference code (Cambridge code, metals code, or inorganic structural code)
82	Internal update code

Journal CODENS

NIST Crystal Data contains the journal CODEN as given by Chemical Abstracts or as assigned by the Crystal Data editors when no published CODEN was available. The journal names have been abbreviated according to conventions of Chemical Abstracts or the Bibliographic Guide for Editors and Authors published by the American Chemical Society.

codenino : Journal CODEN for inorganic data

Columns	Field
1-6	CODEN
8-end	Journal name

codenorg : Journal CODEN for organic data

Columns	Field
1-6	CODEN
8-end	Journal name

CONTACTS

If you have comments or questions about the database, the Standard Reference Data Program would like to hear from you. Also, if you should have any problems with the CD-ROM, please let us know by contacting:

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