Molecular Structures of Gas-Phase Polyatomic Molecules Determined by Spectroscopic Methods

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Spectroscopic data related to the structures of polyatomic molecules in the gas phase have been reviewed, critically evaluated, and compiled. All reported bond distances and angles have been classified as equilibrium (r_e), average (r_z), substitution (r_s), or effective (r_0) parameters, and have been given a quality rating which is a measure of the parameter uncertainty. The surveyed literature includes work from all of the areas of gas-phase spectroscopy from which precise quantitative structural information can be derived. Introductory material includes definitions of the various types of parameters and a description of the evaluation procedure.

Key words: Bond angles; bond distances; gas-phase polyatomic molecules; gas-phase spectroscopy; microwave spectroscopy; molecular conformation; molecular spectroscopy; molecular structure; molecules; structure.

Contents

1. Introduction

Since the first reports of high resolution microwave spectra more than thirty years ago, the microwave spectra of hundreds of molecules have been examined. By far the most common aim of these studies has been the determination of geometrical structural parameters—internuclear distances and angles and nuclear conformations—by analysis of molecular rotational constants. At the same time, precision uv-visible, infrared, and Raman spectroscopy have yielded valuable structural results on relatively small molecules, and more recently molecular beam reasonance methods have played a small but important role. This report is a critical evaluation and compilation of gas-phase structural data for polyatomic molecules determined by these techniques. The literature surveyed in this work covers largely the time period from the late 1940's through 1976 and approximately half-way into 1977.

The critical task of supplying the necessary bibliographic support has been performed by the National Bureau of Standards, although the Londolt-Börnstein tables [1, 2][1] have also been useful in locating pertinent literature. We have tried to include in this survey all polyatomic molecules for which reliable structural data are available for the ground electronic state from spectroscopic studies. Omissions have surely occurred, but it is hoped that they have been held to a minimum.

In the early stages of this project, it had been planned to include diatomic molecules as well as polyatomics. Subsequently, several factors led to the omission of this phase of the evaluation. First, Lovas and Tiemann [3] have recently published a critical review of the spectral data of all those diatomic molecules studied by microwave techniques up to 1974. Secondly, Herzberg and Huber [4] have near completion a comprehensive review of diatomic molecules which will up-to-date the spectral and molecular properties presented in the earlier tables of Herzberg [5]. Since diatomic molecules are of fundamental importance as the cornerstone of structural chemistry, and often provide an important point of comparison for polyatomic molecules, a selection of diatomic distances has been included in an Appendix to this work. In order that nearly all microwave structures might be available in a single source, the Appendix includes all those molecules reviewed by Lovas and Tiemann [3]. Other molecules have been selected for inclusion primarily on the basis of their role as prototypes for the structural units of polyatomic molecules.

Previous compilations containing gas-phase structural data of polyatomic molecules include the tables by Sutton [6], Appendix VIII of Gordy and Cook [7], and Appendix VI of Herzberg [8]. The most recent compilation is that of Callomon et al. [2] covering gas-phase spectroscopic and diffraction data. For diatomic molecules, in addition to the sources mentioned in the previous paragraph, structural data have been compiled by Rosen [9] and have also appeared in the JANAF Thermochemical Tables [10].

The primary aim of the present work is the critical evaluation and compilation of reliable structural data according to a set of relatively well-defined guidelines. The evaluation procedure is described in more detail in subsequent sections, but in general it results in the inclusion of only those structural results that are reliably determined by experimental data and are free of assumptions, intuition, and analogy. For the most part, this means that only those polyatomic molecules for which more than one isotopic species has been studied are included. Exceptions include cases for which unambiguous and non-trivial conformational information could be obtained from a study of only one species.

A second important aspect of the work is that every distance or angle reported has been classified according to a consistent set of operational definitions of the methods of analysis by which the parameters were obtained. These definitions (r_e, r_o, etc.) are described in detail in the following section. Uncertainties in the reported parameters have been reassessed by the reviewers and reported according to a consistent scheme. Finally, when it appeared to be necessary, distances and angles have been recalculated from the reported rotational constants or from the spectra. Because there are many possible slight variations in methods of analysis, reported parameters were replaced by recalculated ones only when the two sets differed by amounts outside the estimated uncertainties.

The format for the presentation of the structural data has been chosen for clarity and simplicity. Distances have been reported in Å (100 pm) units with no more than three decimal digits. This choice is a result of the fact that, except for a relatively small number of polyatomic molecules, experimental and model errors lead to physically meaningless numbers beyond 0.001 Å. For angles, reported in degrees, only one decimal digit has been listed. Parameter uncertainties have been indicated by a letter rating (A, B ...) which defines a range of uncertainty. This scheme was chosen not only for simplicity and clarity, but also to discourage users from placing an unrealistic emphasis upon minor variations in parameters, or an undue reliance upon a precise uncertainty. As described below, the uncertainties in structural parameters for the majority of polyatomic molecules are dominated by rotation-vibration interactions which can be estimated only within certain narrow ranges.

In the next section the various operational definitions of distances and angles are given. Following this, the method of assessing uncertainties is described, and a discussion of the general evaluation procedures is presented. As a final prologue, a brief description is given of the format, content, and organization of the tabulated data.

2. Definitions of Structural Parameters

The Hamiltonian used to analyze the rotational spectra of most molecules consists of some collection of the following terms:

$$\mathcal{H} = \mathcal{H}_R + \mathcal{H}_D + \mathcal{H}_Q + \mathcal{H}_I + \mathcal{H}_{IR} \qquad (1)$$

in which $\mathcal{H}_R$ is the rigid rotator Hamiltonian, $\mathcal{H}_D$ is the contribution from centrifugal distortion, $\mathcal{H}_Q$ describes the nuclear quadrupole interaction, $\mathcal{H}_I$ contains the internal rotation energy, and $\mathcal{H}_{IR}$ describes the interaction of internal and overall rotation. For purposes of distance and angle determination the most important part of (1) is $\mathcal{H}_R$;

$$\mathcal{H}_R = h(AJ_a^2 + BJ_b^2 + CJ_c^2) \qquad (2)$$

in which J_a, J_b and J_c are components of the rotational angular momentum in the directions of the molecule-fixed a, b, and c principal inertial axes, and A, B, and C are rotational constants. The forms of $\mathcal{H}_D$, $\mathcal{H}_Q$, $\mathcal{H}_I$, $\mathcal{H}_{IR}$, and any other possible contributions to the Hamiltonian will not be discussed here; it will be assumed that they have been properly accounted for in each study. Where there

[1] Figures in brackets indicate literature references at the end of section 5.

was question as to whether this was in fact the case, the reviewer either reanalyzed the spectra or omitted the molecule from the compilation.

The rotational constants depend on the vibrational state of the molecules. For molecules for which all the vibrations are harmonic or nearly so, the dependence on vibrational state quantum numbers is as follows:

$$A_v = A_e - \sum_k \alpha_k^{(A)} (v_k + d_k/2) \qquad (3)$$

where $\alpha_k^{(A)}$ is a vibration-rotation parameter, and v_k and d_k are the vibrational quantum number and the degeneracy of the kth vibrational mode, respectively; v stands for $v_1, v_2 \ldots, v_{3N-6}$. In eq (3) A_e is the A rotational constant for the hypothetical equilibrium configuration of the molecule; that is,

$$A_e = h/8\pi^2 I_a^{(e)} \qquad (4)$$

where $I_a^{(e)}$ is the moment of inertia of the molecule about the a-axis when all of the atoms are at equilibrium. Expressions similar to eq (3) and (4) may be written for B_v, B_e, C_v, and C_e. For any vibrational state v,

$$A_v = h/8\pi^2 I_a^{(v)} \qquad (5)$$

in which $I_a^{(v)}$ is an "effective" moment of inertia about the a-axis for molecules in the vibrational state v. Since in any sample most molecules are in the ground vibrational state $v = 0$, the most commonly determined rotational constants are A_0, B_0, and C_0; the corresponding effective moments of inertia are $I_a^{(0)}$, $I_b^{(0)}$, and $I_c^{(0)}$.

The principal moments of inertia may be defined in terms of the eigenvalues of an inertial tensor **P** with components defined as follows:

$$\mathbf{P}_{\alpha\beta} = \sum_{i=1}^{N} m_i \alpha_i \beta_i \qquad (6)$$

in which α_i and β_i are Cartesian x, y, or z coordinates of an atom i of mass m_i. The coordinates are measured from the center of mass of the molecule and the sum is over all the atoms. The principal second moments, taken in the order $P_{aa} \geq P_{bb} \geq P_{cc}$, are the eigenvalues of the tensor **P** and are related to the principal moments of inertia, as follows:

$$I_a = P_{bb} + P_{cc}, \qquad (7a)$$

$$I_b = P_{aa} + P_{cc}, \qquad (7b)$$

$$I_c = P_{aa} + P_{bb}. \qquad (7c)$$

From the definitions in eq (6) and (7) it is clear that the coordinates of the atoms determine the principal moments of inertia. To the extent that the reverse is true—that the moments of inertia determine the coordinates of the atoms—it is possible to calculate distances and angles from experimentally-determined rotational constants.

There are two serious problems in determination of structural parameters from rotational constants. First, there are nearly always many bond distances and angles to be determined and there are only three rotational constants for a single molecular species. It is therefore usually necessary to determine rotational constants for molecules with differing isotopic composition of the nuclei. To high approximation the equilibrium structures of molecules are invariant to isotopic substitution. Thus, equilibrium bond distances and angles, so-called r_e parameters, are determined by adjusting the parameters to give calculated moments of inertia which agree with experimentally-derived equilibrium moments for as many isotopically-substituted species as are necessary.

The second serious problem in structure determination is that it is seldom possible to obtain equilibrium moments of inertia from the spectra. In the most common situation effective rotational constants for the ground vibrational states of one or more isotopic species are available. In addition to the second moment contributions from the sums over the atomic coordinates, effective moments of inertia contain contributions from averaging over the zero-point vibrations and from other vibration-rotation interactions (mainly Coriolis effects). These extra contributions are mass dependent so that the assumption of invariance of structural parameters to isotopic substitution is not valid. Parameters determined by adjusting bond distances and bond angles to give calculated moments of inertia which best fit experimentally derived effective moments of inertia are called effective parameters or r_0 parameters.

In general, equilibrium bond distances and angles determined from different sets of moments of inertia are found to agree within the uncertainties propagated by the experimental uncertainties in the moments. By contrast, effective distances and angles are nearly always strongly dependent on the particular set of moments of inertia used to obtain them. Furthermore, the variations in parameters from set to set may be an order of magnitude or more larger than the propagated experimental uncertainties. As a consequence, uncertainties in effective parameters cannot be deduced from the uncertainties which commonly accompany the results of a least-squares fitting routine. The method used for estimating the uncertainties for effective parameters in the present compilation is described in the next section.

It is possible to reduce the effect of vibration-rotation interactions on the determination of structural parameters from effective moments of inertia by fitting differences in corresponding moments for different isotopic species rather than fitting the moments themselves. This technique is based on the assumption that the vibration-rotation contributions to the moments are very similar for two isotopic species. Since they are mass dependent, however, there is only partial cancellation, so it should not be surprising to find that when the differences in moments of inertia for two isotopic species are very small, the residual differences in vibration-rotation contributions become important.

Differences in moments of inertia may be fit directly by least-squares procedures just as may be done for the moments themselves. However, the simplest procedure is to make use of Kraitchman's equations [11], which are specifically for the case in which two isotopic species of the same molecule differ in isotopic labeling at a single atomic center. One molecule, usually the most common isotopic species, is designated as the parent molecule. Then, according to Kraitchman's equations, the a coordinate of the atom which is isotopically labeled in the substituted molecule is given by the expression [11]

$$a_s = \{(\Delta P_{aa}/\mu)\,[1 + \Delta P_{bb}/(P_{bb} - P_{aa})]\,[1 + \Delta P_{cc}/(P_{cc} - P_{aa})]\}^{1/2}. \quad (8)$$

In eq (8) P_{aa}, P_{bb}, and P_{cc} are effective principal second moments of the parent molecule and

$$\mu = M_P \Delta m/(M_P + \Delta m) \quad (9)$$

in which M_P is the molecular mass of the parent molecule and Δm is the change in mass of the isotopically-substituted atom. Also,

$$\Delta P_{gg} = P'_{gg} - P_{gg} \quad (10)$$

for $g = a, b, c$, in which P'_{gg} is an effective principal second moment of the isotopically substituted molecule. Expressions similar to eq (8) may be written for b_s and c_s by cyclic permutation of subscripts. If the effective moments of inertia are determined for a parent molecule and two singly-substituted species, the coordinates of two atoms may be determined and from them the distance between the atoms. From the data for a parent and three singly-substituted species an interatomic angle can be calculated, etc. Parameters determined by means of Kraitchman's equations are called substitution parameters or r_s parameters [12]. In many structure determinations some of the parameters have been determined by Kraitchman's equations, whereas others are determined by least squares adjustment. In this compilation the former are always labeled r_s parameters. Parameters determined by least squares adjustment to fit only differences in moments of inertia are considered to be r_s parameters also. If, however, any moments of inertia or second moments of inertia are used to determine coordinates of an atom on which no substitution was made, parameters obtained from those coordinates are labeled generally as r_o.

In addition to eq (8) and the corresponding equations for b_s and c_s, it is possible to derive similar equations for multiple substitution at symmetrically equivalent sites [13–15]. Parameters determined from coordinates obtained by these equations are labeled as r_s. It is also possible to derive special forms of the Kraitchman equations for coordinates of atoms which lie in a plane of symmetry or on a symmetry axis [11, 7]. Because a symmetry plane is also a principal inertial plane, the change in the second moment perpendicular to such a plane should vanish for isotopic substitution of an atom in the plane. For substitution on a symmetry axis the changes in both second moments perpendicular to the axis should vanish. For example, for isotopic substitution in the ab inertial plane, ΔP_{cc} should be zero so that $\Delta I_a + \Delta I_b$ should equal ΔI_c. Under these circumstances three combinations of the principal moments of inertia could be used to calculate ΔP_{aa}, as follows:

$$\Delta P_{aa} = (\Delta I_b + \Delta I_c - \Delta I_a)/2 \quad (11a)$$

$$\Delta P_{aa} = \Delta I_b \quad (11b)$$

$$\Delta P_{aa} = \Delta I_c - \Delta I_a \quad (11c)$$

Similar expressions could be written for ΔP_{bb}. Unfortunately, the vibration-rotation contributions do not completely cancel so that ΔP_{cc}, as calculated from effective moments, is never exactly zero for substitution in the ab plane. As a result, the substitution coordinates depend on which of eqs (11) is used to compute ΔP_{aa}. Since no one of these expressions is theoretically preferred, all of the possible combinations should be tested to insure that the parameters reported are representative. Since this has not always been done, the reviewers looked for the possibility of unrepresentative use of Kraitchman's equations. A similar, but more serious problem occurs in the determination of substitution coordinates for molecules which are near oblate symmetric tops. For near oblate tops, P_{aa} is approximately equal to P_{bb} so that the effect of ΔP_{bb} in the second factor of eq (8) is greatly magnified. In the corresponding equation for b_s the effect of ΔP_{cc} is magnified. If either ΔP_{bb} or ΔP_{cc} is small enough that vibration-rotation contributions are a significant fraction of the value, sizable uncertainties in a_s or b_s will result. A procedure for treating this situation by use of data from additional isotopically-labeled species has been described [16].

Examination of the form of eq (8) reveals that the effect of isotopic substitution on the moments of inertia decreases rapidly as the substitution site approaches an inertial plane. This is most easily seen by calculating the change in a coordinate which results from changes in the ΔP_{gg}. In most cases the factors in square brackets in eq (8) contribute an order of magnitude or so less to this change than the first factor. (An exception is the near oblate tops just mentioned.) With these contributions ignored it is found that

$$\delta a_s = \delta \Delta P_{aa}/2\mu a_s. \quad (12)$$

Similar expressions may be derived for δb_s and δc_s. Contributions to $\delta \Delta P_{aa}$ come from experimental uncertainty in the P_{aa} values and from mass-dependent vibration-rotation interactions. It is clear from eq (12) that as $a_s \rightarrow 0$, δa_s gets very large so that the determination of a_s by Kraitchman's equations becomes questionable. If only one coordinate is close to a given plane, it may be determined by the appropriate first moment relation

$$\sum_{i=1}^{N} m_i g_i = 0; g_i = a_i, b_i, \text{ or } c_i. \quad (13)$$

Substitution coordinates are known to satisfy the first moment relations to a good approximation. It is also possible to determine coordinates for atoms close to an inertial plane by the double substitution method of Pierce [17]. In this report coordinates determined either by eq (13) with all g_i but one being substitution coordinates or by Pierce's method are referred to as r_s coordinates.

Substitution parameters were shown by Costain [12] to be considerably less sensitive than effective parameters to the particular set of isotopic species used to determine them. In addition, it is believed that the equilibrium structure is more closely approximated by the r_s structure than by the r_0 structure. For example, Costain [12] has shown that $r_s \simeq \frac{1}{2}(r_0 + r_e)$ for diatomic molecules.

Watson [18] has defined an $I^{(m)}$ moment of inertia as follows:

$$I_g^{(m)} = 2I_g^{(s)} - I_g^{(0)} \quad (14)$$

in which $I_g^{(s)}$ is the moment of inertia about the g-axis calculated from the r_s parameters. The $I^{(m)}$ moments were shown to be equal to equilibrium moments of inertia to first order. Watson [18] has devised a procedure for determining structural parameters from $I^{(m)}$ moments. The resulting bond distances and bond angles are designated as r_m parameters. The r_m procedure is difficult to apply in general because data of very high precision are required for a large number of isotopic species. In addition, the approximation that $I^{(m)} \sim I^{(e)}$ breaks down for very light atoms, so that H-atom parameters cannot be determined by this method. Since the r_m method has been applied to very few molecules, parameters of this type has not been included in this compilation.

Oka [19], Herschbach and Laurie [20], and Toyama, et al. [21], showed that the effective moments of inertia and the moments of inertia of the molecule with all of its atoms in their average positions are related by terms which depend only on the harmonic part of the vibrational potential function. Since the harmonic potential terms are known for many small molecules, a set of moments $I^{(z)}$ for the average configuration can be derived from $I^{(0)}$ values. The bond distances and bond angles derived from the $I^{(z)}$ moments for the ground vibrational state are called average parameters or r_z parameters. Average parameters are mass dependent so that when more than three independent structural parameters must be determined, isotope effects must be estimated. These are typically estimated by assumption of an anharmonicity correction for bond stretching and from computed vibrational amplitudes [22]. In this compilation, no distinction is made between average parameters determined from $I^{(z)}$ moments for a single isotopic species and those determined from $I^{(z)}$ moments for several species with isotope corrections.

TABLE 1. Definitions of structural parameters

Parameter	Definition
r_e (Equilibrium)	Distance or angle between equilibrium nuclear positions.
r_z (Average)	Distance or angle between average nuclear positions in the ground vibrational state.
r_s (Substitution)	Distance or angle calculated from coordinates determined by Kraitchman's equations.
r_0 (Effective)	Distance or angle from coordinates adjusted to give best fit to effective ground state rotational constants.
r_m	Approximate equilibrium distance or angle calculated from coordinates determined by Watson's equations.
r_g	Thermal average value of distance or angle.

It is important to distinguish between r_z parameters—bond distances and angles for the atoms frozen in their average positions—and r_g parameters—the true ground vibrational state average values of distances and angles. The r_g parameters are determined by electron diffraction. It was pointed out by Morino et al. [23] and by Kuchitsu [22] that the difference between an r_z and an r_g distance is the difference between averaging over the molecular motion before or after the distance is calculated. As shown by Kuchitsu, the r_z distance is to good approximation the average of the projection of the distance on the line connecting the nuclei at equilibrium.

The different definitions of structural parameters are summarized in table 1. Comparisons of the different parameters for representative molecules have been given in many places (e.g., in refs. 7, 12, 20, 24, 25, and 26). In addition, many such comparisons appear in data tabulated in this report. Examination of such comparisons shows that differences of several thousandths of an Ångstrom unit in distance and several tenths of a degree in angle should be expected for the different definitions of a given parameter in a molecule. By contrast, the strictly experimental uncertainty is often less than 0.001 Å or 0.1°. As a result, the definition of a reported structural parameter is an important consideration, particularly when parameters from different molecules are compared.

3. Uncertainties

In order to report uncertainties in structural parameters it is necessary to define the basis for the uncertainty estimate. For r_e and r_z parameters, which have well-defined mathematical and physical models, it is sensible to estimate the uncertainties strictly on the basis of the experimental uncertainties of the input data. On the other hand, for r_0 and r_s parameters of polyatomic molecules the operational definitions lead to parameters which are less well-defined physically because of the effects of zero-point vibration-rotation interactions. In this case one would like to know the extent to which these generally unknown molecule-dependent terms contribute to the computed value of the parameters. One way of assessing such contributions would be to compute the values of the parameters (r_0 or r_s) by using several different independent combinations of isotopic data, a procedure which normally leads to a range of values. This range could then serve as a measure of the uncertainty in the computed parameter.

A second way of assessing the uncertainty in r_0 or r_s parameters is to attempt to compute the extent to which vibration-rotation terms cause these parameters to differ from the r_e value. Such a computation cannot be made precisely in the general case; if it could, the more desirable r_e parameter would be obtainable. It is possible, however, to compute an estimate of the general magnitude of the vibration-rotation contributions. Such an approach is the one taken here; the result is an operational definition of the uncertainty which is described below by eqs (20)–(22).

The derivation of eqs (20)–(22) follows from eq (12). For this derivation eq (7) is inverted to give

$$P_{aa}^{(0)} = (I_b^{(0)} + I_c^{(0)} - I_a^{(0)})/2 \qquad (15)$$

and

$$P_{aa}^{(e)} = (I_b^{(e)} + I_c^{(e)} - I_a^{(e)})/2. \qquad (16)$$

Then, a pseudoinertia defect Δ_{aa} is defined to be

$$\Delta_{aa} = 2(P_{aa}^{(e)} - P_{aa}^{(0)}) \qquad (17)$$

from which it follows that, upon isotopic substitution,

$$\Delta P_{aa}^{(0)} = P_{aa}^{(0)\prime} - P_{aa}^{(0)}$$

$$= P_{aa}^{(e)\prime} - P_{aa}^{(e)} - (\Delta'_{aa} - \Delta_{aa})/2. \qquad (18)$$

Therefore, the vibration-rotation contribution to $\delta\Delta P_{aa}$ in eq (12) may be estimated as

$$\delta\Delta P_{aa} = |\,\Delta'_{aa} - \Delta_{aa}\,|/2. \qquad (19)$$

If the value 0.006 u·Å^2 is used for the difference in the pseudoinertia defect upon isotopic substitution, it is found that

$$\delta a_s/\text{Å} = \pm\left|\frac{0.0015}{a_s/\text{Å}}\right|. \qquad (20)$$

A value of 1 u has been assumed for μ. Equation (20) for the uncertainty in the coordinate of an atom derived by application of Kraitchman's equations is known as the Costain rule [27]. Although it has been derived for substitution parameters, it expresses the general insensitivity of the moments of inertia of a molecule to isotopic substitution near a principal inertial plane. The Costain rule should therefore have wide application to the estimation of uncertainties in both r_s and r_0 parameters.

The choice of 0.006 u·Å^2 for $\delta\Delta P_{gg}$ is based on an estimate of a typical difference in pseudoinertial defect upon isotopic substitution. In some cases, particularly for H coordinates, a larger value may be desirable, while for heavy atoms the estimate may be somewhat conservative. The value may also be increased for cases in which the experimental uncertainty in ΔP_{gg} is an appreciable fraction of 0.006 u·Å^2 or in cases in which an unusually large range of coordinate values is obtained by using different combinations of coordinates in Kraitchman's equations.

The unambiguous conversion of uncertainties in atomic coordinates of the r_s or r_0 type to uncertainties in interatomic distances or angles requires more knowledge than is usually available. It is known that the use of the Kraitchman equations can lead to systematic vibration-rotation contributions to the uncertainties in the coordinates [12, 20]. By contrast, in most cases it is probably safe to assume that the experimental contributions to the coordinate uncertainties are distributed randomly. It is possible to compute uncertainties in interatomic parameters by assuming that the contributions to the uncertainties in coordinates from experimental error are random and that the vibration-rotation contributions to each δg_s ($g = a, b, c$) have the same sign as g_s [28]. However, the latter assumption is not always valid and the method requires that the effects of coordinate uncertainties be added absolutely, which probably leads to overstatement of the uncertainties in the distance and angles. In view of these ambiguities it was decided for the purposes of this compilation to use the usual formula for the propagation of random uncertainties to calculate the uncertainties in distances or angles. For the distance between the ith, and jth nuclei this leads to an uncertainty

$$\delta r_{ij} = \left\{\sum_{g=a,b,c}\left[\left(\frac{\partial r_{ij}}{\partial g_i}\right)^2 \delta g_i^2 + \left(\frac{\partial r_{ij}}{\partial g_j}\right)^2 \delta g_j^2\right]\right\}^{1/2}. \qquad (21)$$

In this equation $(\partial r_{ij}/\partial g_i)$ and $(\partial r_{ij}/\partial g_j)$ are calculated from the final structure and δg_i and δg_j for $g = a, b, c$ are obtained by eq (20) or as described in the next paragraph. A corresponding equation for $\delta\theta_{ijk}$ is used to estimate the uncertainties in the angles.

An exception to the use of eq (20) for the determination of the uncertainty in an r_0 or r_s coordinate is made for those coordinates which are calculated by the use of first moment or second moment relations. For example, the uncertainty in a coordinate g_1 which has been calculated by eq (13) is obtained as follows:

$$\delta g_1 = m_1^{-1}\left[\sum_{i=2}^{N}(m_i\,\delta g_i)^2\right]^{1/2} \qquad (22)$$

where the δg_i for $i = 2$ to N are obtained from eq (20).

As mentioned above, eqs (20)–(22) provide the basic operational definition of the uncertainty in an r_s or r_0 bond distance or angle which has been used throughout this work. This definition is intended to be a combined estimate of the contributions of experimental uncertainty and vibration-rotation interaction. It should not, however, be taken too literally. For example, while it is expected that

TABLE 2. Definition of letter symbols for uncertainties

Symbol	Uncertainty range	
	Distance/Å	Angle/degrees
A	≤±0.002	≤±0.2
B	±0.002 – ±0.005	±0.2 – ±0.5
C	±0.005 – ±0.010	±0.5 – ±1.0
D	±0.010 – ±0.020	±1.0 ±2.0
E	±0.020 – ±0.050	±2.0 – ±5.0
X	unable to evaluate, unknown, or unreliable	

the r_e value of the distance or angle will lie within the uncertainty range in many cases, the approximations are such that this cannot be guaranteed.

Uncertainties in equilibrium and average parameters are assigned, as mentioned earlier, by estimating the uncertainties in the input data. The principal contributions to the uncertainty in equilibrium parameters is experimental uncertainties in the measured spectra. The bond distances and bond angles should be isotopically invariant to high approximation. Thus, standard least-squares methods of propagating the uncertainties in the rotational constants to uncertainties in the parameters can be used. The situation for uncertainties in average (r_z) parameters is only slightly different. Here, the principal contributions to uncertainties in the moments of inertia come from experimental uncertainties and from uncertainties in the estimation of $I_g^{(z)}$ from $I_g^{(o)}$. However, additional contributions may come from estimation of isotope effects if moments of inertia from more than one species are required.

In this compilation the numerical values of the uncertainties in the distances or angles are not reported explicitly; a letter rating which corresponds to a range of uncertainty is used instead. The correspondence between the letters used and the uncertainty ranges is given in table 2. The selected ranges for the A, B, C . . . ratings are, of course, arbitrary, but they seem to provide a useful classification of the accuracy of the numbers reported while at the same time they discourage a too-literal interpretation of the uncertainty estimates.

4. Evaluation Procedure

Although each reviewer adopted his own procedure for evaluating the structural parameters in the molecules assigned to him, some steps were common to all of the procedures. These are as follows:

1. The spectral fitting process was examined and uncertainties in the rotational constants were assessed.

2. The method of structural analysis used by the authors was checked for logic and evaluated in a general way. Different definitions were assigned to each of the parameters according to the method of analysis (table 1).

3. For r_e and r_z parameters the errors were established by the errors in the experimental input data. Normally it was found that the published results had a proper assessment of the uncertainties. Numerical uncertainties were converted to letter ratings according to table 2.

4. For r_o and r_s parameters, coordinate uncertainties were established by eq (20) or an equation such as eq (22). These were converted to parameter uncertainties using eq (21) and to letter ratings via table 2. Special methods, such as the "double-substitution" procedure [17], were evaluated as individual cases. For r_o structures, the range of values obtained by using differing data sets provided an additional test of the parameter validity, normally leading to a reduced letter rating.

5. In most cases, structural results were not included if all ratings were X.

6. Studies which reported only conformational results were included when they were unambiguous and non-trivial. Although this represents the least objective aspect of the compilation, such results were deemed to be of sufficient interest and value to merit inclusion.

7. Because of the strong influence of vibration-rotation terms on parameters involving H atoms, such parameters have in most cases been rated no higher than B.

8. In general, the use of parameter assumptions was considered sufficient to invalidate a structure or to lead to X ratings for the dependent parameters. However, in some well-defined cases the uncertainties in computed parameters were assessed according to the plausible uncertainties in the assumed parameters. Since H atom parameter assumptions have a relatively small influence upon heavy atom parameters, such assumptions were normally permitted.

9. The E rating has been used sparingly since a parameter with such a large uncertainty often has little practical validity. Thus a CH bond distance would usually be rated X rather than E in order to indicate its imprecise character. On the other hand, an E rating might provide a useful guideline for certain bond angles or for some of the more uncommon bond lengths.

10. Spot check calculations or complete recalculations of the structure were performed if any results seemed in doubt. Parameters in the original literature were replaced by recalculated values only if the values differed by more than the assigned uncertainty.

5. Description of Tables

Each molecule in this compilation has been identified by its empirical formula according to the conventional scheme. The tables have been arranged so that the inorganic molecules appear first, followed in order by C_1, C_2, C_3, etc. carbon-containing species. Compound names generally follow the standard I.U.P.A.C. or Chemical Abstracts nomenclature schemes, but common names are often included also. Where the empirical formula alone is not sufficient for the identification of the structural parameters, a more conventional structural formula or drawing is included. Additional aid in interpreting the structures is provided by the conventional point group symbol, which is listed for each molecule above the data table.

Structural parameters for each molecule are tabulated according to their operational definition, viz., substitution (r_s), equilibrium (r_e), effective (r_0), or average (r_z), and are separated into distance and angle categories. As a general rule, r_e, r_s, and r_z parameters are always listed when available; r_0 values are normally included only if one of the more reliable types can not be obtained from the experimental data. All distance values are in Å (100 pm) units and angles are in degrees. Explanatory comments and footnotes follow the tabulated parameters, and finally the original literature sources are listed. In most cases only those sources have been referenced which are necessary to obtain the reported structure.

All structural data in this compilation refer to the ground electronic state, which for most polyatomic molecules implies a totally symmetrical orbital state with a spin multiplicity of unity. For those few molecules whose ground states do not fall in this category, the standard term symbol has been listed below the table. Except for a few cases as noted, all structural parameters refer to the normal (most abundant) isotopic species, although the equilibrium parameters are expected to be isotopically invariant.

Acknowledgments

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[2] Callomon, J. H., Hirota, E., Kuchitsu, K., Lafferty, W. J., Maki, A. G., and Pote, C. S., "Structure Data of Free Polyatomic Molecules," in Landolt-Bornstein, New Series, Group II. Volume 7, Editor-in-Chief, K. H. Hellwege, Springer-Verlag, Berlin (1976).

[3] Lovas, F. J., and Tiemann, E., J. Phys. Chem. Ref. Data **3**, 609 (1974).

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[14] Nygaard, L., J. Mol. Spectrosc. **62**, 292 (1976).

[15] Li, Y. S., Kiser, K. L., and Durig, J. R., J. Mol. Spectrosc. **42**, 430 (1972).

[16] Kuczkowski, R. L., Gillies, C. W., and Gallaher, K. L., J. Mol. Spectrosc. **60**, 361 (1976).

[17] Pierce, L., J. Mol. Spectrosc. **3**, 575 (1959).

[18] Watson, J. K. G., J. Mol. Spectrosc. **48**, 479 (1973).

[19] Oka, T., J. Phys. Soc. Japan **15**, 2274 (1960).

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[21] Toyama, M., Oka, T., and Morino, Y., J. Mol. Spectrosc. **13**, 193 (1964).

[22] Kuchitsu, K., and Cyvin, S. J., *Molecular Structures and Vibrations*, S. J. Cyvin, Ed., Elsevier, Amsterdam (1972), Chap. 12.

[23] Morino, Y., Kuchitsu, K., and Oka, T., J. Chem. Phys. **36**, 1108 (1962).

[24] Kuchitsu, K., J. Chem. Phys. **49**, 4456 (1968).

[25] Lide, D. R., Jr., *MTP International Review of Science, Physical Chemistry Series Two*, A. D. Buckingham, Ed., Butterworths, London (1975), Vol. 2, Chap. 1.

[26] Schwendeman, R. H., "Critical Evaluation of Chemical and Physical Structural Information," D. R. Lide and M. A. Paul, Eds., National Academy of Sciences, Washington (1974), p. 94.

[27] Costain, C. C., Trans. Am. Cryst. Assoc. **2**, 157 (1966).

[28] Tobiason, F. L., and Schwendeman, R. H., J. Chem. Phys. **40**, 1014 (1964).

Appendix: Selected Diatomic Molecule Distances[a]

Molecule	r_o	r_e	Molecule	r_o	r_e	Molecule	r_o	r_e
AgBr	2.395	2.393	ClCs	2.910	2.906	HN	1.045	1.035
AgCl	2.284	2.281	ClF	1.632	1.628	HO	0.980	0.971
AgF	1.987	1.983	ClGa	2.205	2.202	HP	1.433*	
AgI	2.547	2.545	ClH	1.284	1.275	HS	1.355	1.345*
AlBr	2.298	2.295	ClI	2.324	2.321	HSi	1.531	1.520*
AlCl	2.133	2.130	ClIn	2.404	2.401	H_2	0.751	0.741*
AlF	1.658	1.654	ClK	2.671	2.667	IIn	2.756	2.754
AlI	2.540	2.537	ClLi	2.027	2.021	IK	3.051	3.048
BF	1.267	1.263	ClNa	2.365	2.361	ILi	2.398	2.392
BH	1.247	1.236*	ClO	1.573	1.569	INa	2.715	2.711
BN	1.286	1.281*	ClRb	2.790	2.787	IRb	3.180	3.177
BO	1.210	1.204*	ClTl	2.488	2.485	ITl	2.815	2.814
B_2	1.594	1.590*	Cl_2	1.991	1.988*	I_2	2.669	2.667*
BaO	1.942	1.940	CsF	2.347	2.345	Li_2	2.680	2.673*
BrCl	2.139	2.136	CsI	3.318	3.315	NO	1.154	1.151
BrCs	3.075	3.072	CuF	1.749	1.745	NP	1.494	1.491
BrF	1.759	1.756	FGa	1.778	1.774	NS	1.497	1.494
BrGa	2.355	2.352	FH	0.926	0.917	N_2	1.100	1.098*
BrH	1.424	1.415	FI	1.913	1.910	OP	1.476	1.474*
BrI	2.489	2.485	FIn	1.989	1.985	OPb	1.925	1.922
BrIn	2.545	2.543	FK	2.176	2.171	OS	1.484	1.481
BrK	2.824	2.821	FLi	1.570	1.564	OSi	1.512	1.510
BrLi	2.176	2.170	FN	1.321	1.317*	OSn	1.835	1.833
BrNa	2.506	2.502	FNa	1.931	1.926	O_2	1.211	1.208
BrO	1.721	1.717	FRb	2.274	2.270	P_2	1.896	1.894*
BrRb	2.948	2.945	FS	1.601		PbS	2.289	2.287
TlBr	2.620	2.618	FTl	2.088	2.084	PbSe	2.404	2.402
CBr		1.821*	F_2	1.417*		PbTe	2.596	2.595
CCl	1.649	1.645*	GaI	2.577	2.575	SSi	1.932	1.929
CF	1.276	1.272*	GeO	1.627	1.625	SSn	2.211	2.209
CH	1.131	1.120*	GeS	2.014	2.012	S_2	1.892	1.889*
CN	1.175	1.172*	GeSe	2.136	2.135	SeSi	2.060	2.058
CO	1.131	1.128	GeTe	2.342	2.340	SeSn	2.327	2.326
CS	1.538	1.535	HI	1.620	1.609	Si_2	2.249	2.246*
CSe	1.679	1.676	HLi	1.604	1.595[b]	SnTe	2.524	2.523
C_2	1.246	1.243*						

[a] Distances are expected to have an accuracy of 0.001 Å or better. Values indicated by an asterisk have been obtained from Rosen [9], the remaining values from Lovas and Tiemann [3].

[b] In this case the values are for the deuterated species, ^{2}HLi.

Structural Data Tables

Inorganic Molecules

Aluminum Dihydride

AlH_2 C_{2v}

Bond	Effective	Angle	Effective
AlH	1.59 E	HAlH	119 E

[1] G. Herzberg, *Electronic Spectra of Polyatomic Molecules*, D. Van Nostrand Co. Inc., Princeton, N.J., U.S.A., Table 62, 1966.

Argon–Hydrogen chloride (1/1)

ArClH Ar·ClH C_s

Bond	Effective	Angle	Effective
HCl	1.284 (assumed)	ArClH	41.5 X
ArCl	4.01 X		

[1] S. E. Novick, P. Davies, S. Harris and W. Klemperer, J. Chem. Phys. **59**, 2273 (1973).

Hydrogen Argon (1/1)

ArH_2 $Ar \cdot H_2$ Undefined

Bond	Effective
Mean distance between center of mass of H_2 and Ar atom.	3.94 X

[1] A. R. W. McKellar and H. L. Welsh, J. Chem. Phys. **55**, 595 (1971).

Arsenic tribromide

$AsBr_3$ C_{3v}

Bond	Effective	Average	Angle	Effective	Average
AsBr	2.323 B	2.324 B	BrAsBr	99.8 B	99.7 B

[1] A. G. Robiette, J. Mol. Struct. **35**, 81 (1976).

Arsenic Trifluoride (Trifluoroarsine)

AsF_3 C_{3v}

Bond	Effective	Angle	Effective
AsF	1.712 X	FAsF	102 X

Only one isotopic species studied.

[1] P. Kosliuk and S. Geschwind, J. Chem. Phys. **21**, 828 (1953).

Arsino

AsH_2 C_{2v}

Bond	Effective	Angle	Effective
AsH	1.518 C	HAsH	90.7 B

Ground electronic state is $^2B_1$.

[1] R. N. Dixon, G. Duxbury and H. M. Lamberton, Proc. Roy. Soc. (London) **A305**, 271 (1968).

Arsine

AsH_3 C_{3v}

Bond	Effective	Equilibrium	Angle	Effective	Equilibrium
AsH	1.520 A	1.511 A	HAsH	92.0 A	92.1 A

[1] W. B. Olson, A. G. Maki and R. L. Sams, J. Mol. Spectrosc. **55**, 252 (1975).
[2] F. Y. Chu and T. Oka, J. Chem. Phys. **60**, 4612 (1974).
[3] K. Sarka, D. Papousek and K. N. Rao, J. Mol. Spectrosc. **37**, 1 (1971).
[4] P. Helminger, E. L. Beeson and W. Gordy, Phys. Rev. **A3**, 122 (1971).

Boron chloride difluoride

$BClF_2$ $ClBF_2$ C_{2v}

Bond	Substitution	Effective	Angle	Effective
BCl	1.728 C		FBF	118.1 C
BF		1.315 C		

[1] H. W. Kroto and M. Maier, J. Mol. Spectrosc. **65**, 280 (1977).

Difluoroborane

BF_2H C_{2v}

Bond	Substitution	Effective	Angle	Effective
BH	1.189 C		FBF	118.3 C
BF		1.311 C		

[1] T. Kasuya, W. J. Lafferty and D. R. Lide, J. Chem. Phys. **48**, 1 (1968).

Difluorohydroxyborane

BF_2HO F_2BOH C_s

Bond	Substitution	Effective	Angle	Effective
OH	0.94 C		BOH	114 C
BO		1.34 D	FBO	123 C
BF		1.31 D	FBF	118 C

[1] H. Takeo and R. F. Curl, J. Chem. Phys. **56**, 4314 (1972).

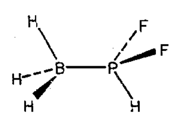
1,1-Difluoroboranamine (Aminodifluoroborane)

BF_2H_2N BF_2NH_2 C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
BF		1.325 C	FBF		117.9 B
BN		1.402 D	NHN	116.9 B	
NH	1.003 B				

[1] F. J. Lovas and D. R. Johnson, J. Chem. Phys. **59**, 2347 (1973).

Difluorophosphine Borane



BF_2H_4P C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
PH		1.409 C	H_aBH_a	112.7 C	
PF		1.552 C	H_aBH_s	115.9 C	
PB		1.832 D	PBH_s		109.9 B
BH_a	1.226 B		PBH_a		99.9 B
BH_s	1.200 C		BPH		120.1 C
			BPF		117.7 B
			FPF		100.0 C
			FPH		98.6 B

Subscripts s and a refer to in and out of the plane of symmetry, respectively.

[1] J. P. Pasinski and R. L. Kuczkowski, J. Chem. Phys., **54**, 1903 (1971).

Boron Fluoride Oxide (Difluoroboroxy)

BF_2O F_2BO C_{2v}

Bond	Effective	Angle	Effective
BF	1.30 E	FBF	126 E
BO	1.40 E		

Ground electronic state is $^2B_2$.

[1] C. W. Mathews, J. Mol. Spectrosc. **19**, 203 (1966).

Boron Trifluoride (Trifluoroborane)

BF_3 D_{3h}

Bond	Effective	Equilibrium
BF	1.310 B	1.307 B

[1] S. G. W. Ginn, J. K. Kenny and J. Overend, J. Chem. Phys. **48**, 1571 (1968).
[2] C. W. Brown and J. Overend, Can. J. Phys. **46**, 977 (1968).

Phosphine-trifluoroborane

BF_3H_3P $F_3B\text{-}PH_3$ C_{3v}

Bond	Effective	Angle	Effective
PB	1.92 X	FBP	107. X
BF	1.37 X	FBF	112. X

PH distance assumed to be 1.40 Å and HPB angle assumed to be 117°.

[1] J. D. Odom, V. F. Kalasinsky, and J. R. Durig, Inorg. Chem. **14**, 2837 (1975).

Phosphorus Trifluoride-Borane

BF_3H_3P F_3PBH_3 C_{3v}

Bond	Substitution	Effective	Angle	Substitution	Effective
BH	1.207 B		HBH	115.1 C	
PF		1.538 D	FPF		99.8 D
PB		1.836 D			

[1] R. L. Kuczkowski and D. R. Lide, Jr., J. Chem. Phys. **46**, 357 (1967).

Thioxoborane(3) (Thioborane)

BHS HBS $C_{\infty v}$

Bond	Substitution
BH	1.169 A
BS	1.599 A

[1] E. F. Pearson and R. U. McCormick, J. Chem. Phys. **58**, 1619 (1973).

Borane(2)

BH_2 C_{2v}

Bond	Effective	Angle	Effective
BH	1.181 C	HBH	131 C

Ground state is $^2B_1$.
[1] G. Herzberg and J. W. C. Johns, Proc. Roy. Soc. (London) **A298**, 142 (1967).

Phosphine–Borane

BH_6P H_3BPH_3 C_{3v}

Bond	Substitution	Angle	Substitution
BP	1.937 B	PBH	103.6 B
BH	1.212 B	BPH	116.9 B
PH	1.399 B	HBH	114.6 B
		HPH	101.3 B

[1] J. R. Durig, Y. S. Li, L. A. Carreira, and J. D. Odom, J. Amer. Chem. Soc. **95**, 2491 (1973).

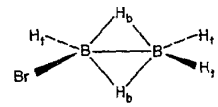
Boron Dioxide

BO_2 OBO $D_{\infty h}$

Bond	Effective
BO	1.265 A

Ground electronic state is $^2\Pi_g$.
[1] J. W. C. Johns, Can. J. Phys. **39**, 1738 (1961).

Bromodiborane(6)

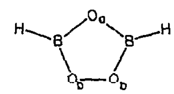


B_2BrH_5 C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
BB	1.773 B		BBBr	121.4 C	
BBr	1.930 B		BBH_t		119.9 X
H_bH_b		1.954 X	H_bBH_b		95.6 X
BH_t		1.196 X	BH_bB		84.4 X

[1] A. C. Ferguson and C. D. Cornwell, J. Chem. Phys. **53**, 1851 (1970).

1,2,4,3,5-Trioxadiborolane

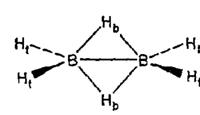


$B_2H_2O_3$ C_{2v}

Bond	Substitution	Angle	Substitution
BH	1.182 B	BOB	104.0 C
BO_a	1.380 B	OBO	113.0 C
BO_b	1.365 B	BOO	105.0 C
O_bO_b	1.470 A	HBO_a	126.3 C

[1] W. V. F. Brooks, C. C. Costain and R. F. Porter, J. Chem. Phys. **47**, 4186 (1967).

Diborane(6)

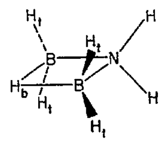


B_2H_6 D_{2h}

Bond	Effective	Angle	Effective
B···B	1.763 C	H_tBH_t	121.0 C
$B\text{-}H_t$	1.201 C	H_bBH_b	96.2 C
$B\text{-}H_b$	1.320 C		

[1] W. J. Lafferty, A. G. Maki and T. D. Coyle, J. Mol. Spectrosc. **33**, 345 (1970).

Aminodiborane

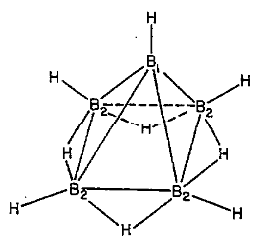


B_2H_7N C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
BB	1.916 B		BNB	75.9 A	
BN	1.558 B		BH_bB	90.0 B	
BH_b	1.355 C		H_tBH_t	121.0 B	
BH_t	1.193 B		NBH_t	113.7 B	
NH		1.005 C	HNH		111.0 D

[1] K. K. Lau, A. B. Burg, and R. A. Beaudet, Inorg. Chem. **13**, 2787 (1974).

Pentaborane (9)



B_5H_9 C_{4v}

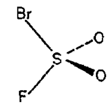
Bond	Effective
B_1B_2	1.687 C
B_2B_2	1.800 C

Hydrogen atoms are not uniquely determined, but data are consistent with five single BH bonds and four bridging hydrogens as shown.

[1] H. J. Hrostowski and R. J. Myers, J. Chem. Phys. **22**, 262 (1954).

[2] H. J. Hrostowski, R. J. Myers and G. C. Pimentel, J. Chem. Phys. **20**, 518 (1952).

Sulfuryl bromide fluoride



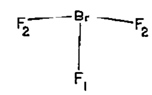
$BrFO_2S$ C_s

Bond	Effective	Angle	Effective
SBr	2.155 X	FSBr	100.6 X

SO, SF, and OSO were assumed to be 1.407, 1.560, and 123.7, respectively.

[1] J. M. Raley and J. E. Wollrab, J. Mol. Spectrosc. **48**, 100 (1973).

Bromine fluoride (Bromine trifluoride)



BrF_3 C_{2v}

Bond	Effective	Angle	Effective
BrF_1	1.721 C	F_1BrF_2	86.2 C
BrF_2	1.810 B		

[1] D. W. Magnuson, J. Chem. Phys. **27**, 223 (1957).

Bromotrifluorosilane

BrF_3Si SiF_3Br C_{3v}

Bond	Effective	Angle	Effective
SiF	1.560 B	FSiF	108.5 D
SiBr	2.153 D		

Bond distances determined by assuming the value for FSiF.

[1] J. Sheridan and W. Gordy, J. Chem. Phys. **19**, 965 (1951).

Sulfur bromide fluoride (Sulfur pentafluoride bromide)

BrF_5S $BrSF_5$ C_{4v}

Bond	Effective
SBr	2.190 X
SF	1.597 X

Angle F(eq)SF(ax) was assumed to be 88.0°, and all SF bond lengths were assumed to be equal.

[1] E. W. Neuvar and A. W. Jache, J. Chem. Phys. **39**, 596 (1963).

Bromogermane

$BrGeH_3$ $BrGeH_3$ C_{3v}

Bond	Effective	Substitution	Angle	Effective
Ge–H	1.535 D		HGeH	111.9 D
Ge–Br		2.297 B		

The substitution distance derived in Ref. 1 was combined with the A_0 value obtained in Ref. 2 by use of the zeta sum rule to calculate the molecular parameters.

[1] S. N. Wolf and L. C. Krisher, J. Chem. Phys. **56**, 1040 (1972).
[2] K. H. Rhee and M. K. Wilson, J. Chem. Phys. **43**, 333 (1965).

Bromosilylene

BrHSi HSiBr C_s

Bond	Effective	Angle	Effective
SiBr	2.231 B	HSiBr	102.9 C

SiH distance assumed (1.561 Å).

[1] G. Herzberg and R. D. Verma, Can. J. Phys. **42**, 395 (1964).

Bromosilane

BrH_3Si $BrSiH_3$ C_{3v}

Bond	Substitution	Angle	Substitution
SiBr	2.210 B	HSiBr	107.9 B
SiH	1.481 B		

[1] R. Kawley, P. M. McKinney, and A. G. Robiette, J. Mol. Spectrosc. **34**, 390 (1970).

Bromostannane

BrH_3Sn $BrSnH_3$ C_{3v}

Bond	Substitution	Effective	Angle	Effective
SnBr	2.469 A		HSnBr	106 C
SnH		1.76 X		

[1] S. N. Wolf, L. C. Krisher, and R. A. Gsell, J. Chem. Phys. **54**, 4605 (1971).

Nitrosyl Bromide

BrNO C_s

Bond	Effective	Angle	Effective
NO	1.146 D	BrNO	114.5 C
NBr	2.140 C		

[1] D. J. Millen and D. Mitra, Trans. Faraday Soc. **65**, 1975 (1969).

Fluorotribromosilane

Br_3FSi $FSiBr_3$ C_{3v}

Bond	Effective	Angle	Effective
SiBr	2.171 X	BrSiBr	111.6 X

SiF = 1.560 was assumed.

[1] M. Mitzlaff, R. Holm and H. Hartmann, Z. Naturforsch. **23a**, 1819 (1968).

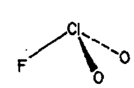
Tribromosilane

Br_3HSi Br_3SiH C_{3v}

Bond	Effective	Angle	Effective
SiH	1.494 C	BrSiBr	111.6 E
SiBr	2.170 E		

[1] M. Mitzlaff, R. Holm, and H. Hartmann, Z. Naturforsch. **23a**, 65 (1968).

Chloryl fluoride

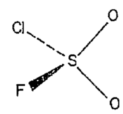


$ClFO_2$ C_s

Bond	Substitution	Angle	Substitution
ClF	1.696 B	OClO	115.2 A
ClO	1.418 B	FClO	101.7 A

[1] C. R. Parent and M. C. L. Gerry, J. Mol. Spectrosc. **49**, 343 (1974).

Sulfuryl chloride fluoride



$ClFO_2S$ C_s

Bond	Effective	Angle	Effective
SO	1.408[a]	OSO	123.7 X
SF	1.550 X	FSCl	99.0[a]
SCl	1.985 X	OSF	107.5 X
		OSCl	107.5 X

[a] Assumed values.

[1] C. S. Holt and M. C. L. Gerry, Chem. Phys. Lett. 9, 621 (1971).

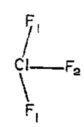
Phosphorous chloride difluoride (Chlorodifluorophosphine)

ClF_2P PF_2Cl C_s

Bond	Effective	Angle	Effective
PF	1.571 B	FPF	97.3 B
PCl	2.030 C	FPCl	99.2 C

[1] A. H. Brittain, J. E. Smith and R. H. Schwendeman, Inorg. Chem. 11, 39 (1972).

Chlorine Fluoride



ClF_3 C_{2v}

Bond	Effective	Angle	Effective
ClF_1	1.598 B	F_1ClF_2	87.5 B
ClF_2	1.698 B		

[1] D. F. Smith, J. Chem. Phys. 21, 609 (1953).

Chlorotrifluorogermane

ClF_3Ge GeF_3Cl C_{3v}

Bond	Effective	Angle	Effective
GeF	1.688 D	FGeF	107.5 E
GeCl	2.067 C		

[1] W. E. Anderson, J. Sheridan and W. Gordy, Phys. Rev. 81, 819 (1951).

Chlorotrifluorosilane

ClF_3Si SiF_3Cl C_{3v}

Bond	Effective
SiF	1.560 C
SiCl	1.989 E

Bond distances obtained by assuming FSiF = 108.5 ± 2°.

[1] J. Sheridan and W. Gordy, J. Chem. Phys. 19, 965 (1951).

Chlorine pentafluoride

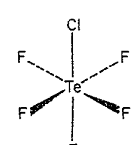
ClF_5 C_{4v}

Bond	Effective	Angle	Effective
ClF	1.65 X	$F_{ax}ClF_{eq}$	86.5 X
		$F_{eq}ClF_{eq}$	89.9 X

The ClF_{ax} and ClF_{eq} distances have been assumed to be equal.

[1] H. K. Bodenseh, W. Hüttner, and P. Nowicki, Z. Naturforsch. 31a, 1638 (1976).
[2] P. Goulet, R. Jurek, and J. Chanussot, J. de Phys. 37, 495 (1976).
[3] R. Jurek, P. Suzeau, J. Chanussot, and J. P. Champion, J. de Phys. 35, 533 (1974).

Tellurium pentafluoride chloride



ClF_5Te C_{4v}

Bond	Substitution	Effective	Angle	Substitution	Effective
TeCl	2.250 B		$F_{eq}TeF_{ax}$		88.3 X
TeF		1.831 X			

The TeF_{eq} distance has been assumed equal to the TeF_a distance.

[1] A. C. Legon, J. Chem. Soc., Faraday Trans. 69, 29 (1973).

Tungsten pentafluoride chloride

ClF_5W $ClWF_5$ C_{4v}

Bond	Substitution	Effective	Angle	Effective
WCl	2.252 B		θ^b	88.7 X
WF[a]		1.836 X		

[a] All WF bonds assumed equal.
[b] F_{axial} $WF_{equatorial}$ angle.

[1] A. C. Legon, Trans Faraday Soc. **65**, 2595 (1969).

Hypochlorous acid

ClHO HOCl C_s

Bond	Substitution	Angle	Substitution
OH	0.967 C	HOCl	102.4 C
OCl	1.690 A		

[1] A. M. Mirri, F. Scappini and G. Cazzoli, J. Mol. Spectrosc. **38**, 227 (1971).
[2] D. C. Lindsey, D. G. Lister and D. J. Millen, Chem. Comm. **1969**, 950 (1969).
[3] R. A. Ashby, J. Mol. Spectrosc. **23**, 439 (1967).

Chlorosilylene

ClHSi HSiCl C_s

Bond	Effective	Angle	Effective
SiH	1.561 C	HSiCl	102.8 B
SiCl	2.064 B		

[1] G. Herzberg and R. D. Verma, Can. J. Phys. **42**, 395 (1964).

Chloramide (Monochloramine)

ClH_2N $ClNH_2$ C_s

Bond	Substitution	Angle	Substitution
NH	1.017 C	HNCl	103.7 B
NCl	1.748 A	HNH	107.4 D

[1] G. Cazzoli, D. G. Lister and P. G. Favero, J. Mol. Spectrosc. **42**, 286 (1972).
[2] G. E. Moore and R. M. Badger, J. Amer. Chem. Soc. **74**, 6076 (1952).

Chlorosilane

ClH_3Si H_3SiCl C_{3v}

Bond	Substitution	Effective	Angle	Substitution	Effective
SiCl	2.048 A	2.049 A	HSiCl	107.9 B	108.7 B
SiH	1.482 B	1.485 B			

[1] R. Kewley, P. M. McKinney and A. G. Robiette, J. Mol. Spectrosc. **34**, 390 (1970).

Chlorostannane

ClH_3Sn H_3SnCl C_{3v}

Bond	Substitution	Effective
SnCl	2.327 A	
SnH		1.70 X[a]

[a] Value obtained by assuming methyl group to be tetrahedral.

[1] L. C. Krisher, R. A. Gsell and J. M. Bellama, J. Chem. Phys. **54**, 2287 (1971).

Nitrosyl chloride

ClNO O=N—Cl C_s

Bond	Substitution	Angle	Substitution
NO	1.139 C	ONCl	113.3 C
NCl	1.975 B		

[1] D. J. Millen and J. Pannell, J. Chem. Soc. **1961**, 1322 (1961).

Nitryl chloride

$ClNO_2$ C_{2v}

Bond	Effective	Angle	Effective
NCl	1.840 B	ONO	130.6 C
NO	1.202 B		

[1] D. J. Millen and K. M. Sinnott, J. Chem. Soc. **1958**, 350.
[2] L. Clayton, Q. Williams and T. L. Weatherly, J. Chem. Phys. **30**, 1328 (1959), Errata, J. Chem. Phys., **31**, 554 (1959).
[3] T. Oka and Y. Morino, J. Mol. Spectrosc. **11**, 349 (1963).

Thiazyl chloride

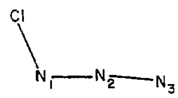
ClNS N≡S—Cl C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
NS	1.450 A	1.452 B	NSCl	117.7 A	117.9 B
SCl	2.161 A	2.161 B			

The effective structure is an average of that determined in three independent ways.

[1] T. Beppu, E. Hirota and Y. Morino, J. Mol. Spectrosc. **36**, 386 (1970).

Chlorine azide



ClN_3 C_s

Bond	Substitution	Angle	Substitution
ClN_1	1.745 C	ClN_1N_2	108.7 C
N_1N_2	1.252 C	$N_1N_2N_3$	171.9 C
N_2N_3	1.133 C		

[1] R. L. Cook and M. C. L. Gerry, J. Chem. Phys. **53**, 2525 (1970).

Chlorine dioxide

ClO_2 OClO C_{2v}

Bond	Substitution	Average	Angle	Substitution	Average
ClO	1.471 B	1.476 B	OClO	117.6 B	117.5 B

Ground state is $^2B_1$.

[1] A. H. Clark, J. Mol. Struct. **7**, 485 (1971).
[2] F. R. Curl, Jr., R. F. Heidelberg and J. L. Kinsey, Phys. Rev. **125**, 1993 (1962).
[3] R. F. Curl, Jr., J. L. Kinsey, J. G. Baker, J. C. Baird, G. R. Bird, R. F. Heidelberg, T. M. Sugden, D. R. Jenkins and C. N. Kenney, Phys. Rev. **121**, 1119 (1961).

Chlorotrioxorhenium

ClO_3Re $ClReO_3$ C_{3v}

Bond	Effective	Angle	Effective
ReO	1.702 B	ClReO	109.4 B
ReCl	2.229 B		

[1] E. Amble, S. L. Miller, A. L. Schawlow and C. H. Townes, J. Chem. Phys. **20**, 192 (1952).
[2] J. F. Lotspeich, A. Javan and A. Engelbrecht, J. Chem. Phys. **31**, 633 (1959).

Dichlorosilane

Cl_2H_2Si C_{2v}

Bond	Substitution	Angle	Substitution
SiCl	2.033 A	ClSiCl	109.7 B
SiH	1.480 D	HSiH	111.3 C

Hydrogen parameters are not strictly substitution parameters, but should be nearly so.

[1] R. W. Davis and M. C. L. Gerry, J. Mol. Spectrosc. **60**, 117 (1976).

Dichlorine oxide

Cl_2O ClOCl C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
ClO	1.700 A	1.700 A	ClOCl	110.9 B	110.9 B

[1] G. E. Herberick, R. H. Jackson and D. J. Millen, J. Chem. Soc. **1966**, 1156 (1966).

Sulfur dichloride

Cl_2S C_{2v}

Bond	Substitution	Average	Effective
ClS	2.014 A	2.015 A	2.014 A

Angle	Substitution	Average	Effective
ClSCl	102.6 A	102.7A	102.7 A

[1] R. W. Davis and M. C. L. Gerry, J. Mol. Spectrosc. **65**, 455 (1977).
[2] J. L. Murray, W. A. Little, Q. Williams and T. L. Weatherby, J. Chem. Phys. **65**, 985 (1976).

Trichlorofluorosilane

Cl_3FSi $FSiCl_3$ C_{3v}

Bond	Effective	Angle	Effective
SiF	1.520 B	FSiCl	109.5 B
SiCl	2.019 B	ClSiCl	109.4 B

[1] R. Holm, M. Mitzloff and H. Hartmann, Z. Naturforschg. **22a**, 1287 (1967).

Trichlorogermane

Cl_3GeH — $HGeCl_3$ — C_{3v}

Bond	Effective	Angle	Effective
GeH	1.55 E	ClGeCl	2.114 A
GeCl	2.114 A		

[1] P. Venkateswarlu, R. C. Mockler, and W. Gordy, J. Chem. Phys. **21**, 1713 (1953).

Trichlorosilane

Cl_3HSi — $HSiCl_3$ — C_{3v}

Bond	Substitution	Effective	Angle	Substitution	Effective
HSi	1.465 A	1.47 X	HSiCl	108.3 B	109.5 B
ClSi	2.019A	2.021 A	ClSiCl	110.6 B	109.4 B

[1] R. Mockler, J. H. Bailey, and W. Gordy, J. Chem. Phys. **21**, 1710 (1953).
[2] M. Mitzlaff. R. Holm and H. Hartmann, Z. Naturforschg. **22a**, 1415 (1967).

Nitrogen trichloride

Cl_3N — NCl_3 — C_{3v}

Bond	Substitution	Effective	Angle	Substitution	Effective
NCl	1.754 A	1.759 A	ClNCl	107.8 A	107.4 A

[1] G. Gazzoli, P. G. Favero, and A. Dal Borgo, J. Mol. Spectrosc. **50**, 82 (1974).

Phosphoryl chloride

Cl_3OP — C_{3v}

Bond	Effective	Angle	Substitution
PO	1.455 D	ClPCl	103.7 C
PCl	1.989 C		

[1] Y. S. Li, M. M. Chen and J. R. Durig, J. Mol. Struct. **14**, 261 (1972).

Vanadyl(V) chloride

Cl_3OV — C_{3v}

Bond	Effective	Angle	Effective
VO	1.587 C	ClVCl	111.6 B
VCl	2.133 B		

The structural parameters were recalculated from the reported rotational constants.

[1] K. Karakida and K. Kuchitsu, Chem. Lett. 293 (1972).

Phosphorous Trichloride

Cl_3P — PCl_3 — C_{3v}

Bond	Effective	Angle	Effective
PCl	2.043 B	ClPCl	100.1 C

[1] P. Kisliuk and C. H. Townes, J. Chem. Phys. **18**, 1109 (1950).

Cesium Hydroxide

CsHO — CsOH — $C_{\infty v}$

Bond	Effective	Equilibrium
CsO	2.403 C	2.391 A
OH	0.920 C	0.960 C

[1] D. R. Lide, Jr. and R. L. Kuczkowski, J. Chem. Phys. **46**, 4768 (1967).
[2] D. R. Lide, Jr. and C. Matsumura, J. Chem. Phys. **50**, 3080 (1969).

Fluorogermane

$FGeH_3$ — C_{3v}

Bond	Substitution	Effective	Angle	Effective
GeF	1.730 E		HGeH	113.0 D
GeH		1.522 D		

[1] L. C. Krisher, J. A. Morrison, W. A. Watson, J. Chem. Phys. **57**, 1357 (1972).
[2] K. H. Rhee and M. K. Wilson, J. Chem. Phys. **43**, 333 (1965).

Fluoroamidogen

FHN HNF C_s

Bond	Effective	Angle	Effective
NF	1.37 C	HNF	105 C

Ground electronic state is $^2A''$.
NH distance assumed (1.06 Å).

[1] C. M. Woodman, J. Mol. Spectrosc. 33, 311 (1970).

Hypofluorous acid

FHO HOF C_s

Bond	Effective	Angle	Effective
OH	0.966 D	HOF	96.8 C
OF	1.442 B		

[1] E. F. Pearson and H. Kim, J. Chem. Phys. 57, 4230 (1972).
[2] H. Kim, E. F. Pearson and E. H. Appelman, J. Chem. Phys. 56, 1 (1972).

Fluorosilane

FH_3Si SiH_3F C_{3v}

Bond	Substitution	Average	Effective
SiF	1.590 B	1.596 B	1.593 B
SiH	1.471 B	1.480 B	1.485 C

Angle	Substitution	Average	Effective
HSiF	107.9 B	108.4 B	108.4 C

[1] A. H. Sharbaugh, V. G. Thomas and B. S. Pritchard, Phys. Rev. 78, 64 (1950).
[2] B. Bak, J. Bruhn and J. Rastrup-Andersen, J. Chem. Phys. 21, 752 (1953).
[3] C. Georghiou, J. G. Baker and S. R. Jones, J. Mol. Spectrosc. 63, 89 (1976).
[4] A. G. Robiette, C. Georghiou and J. G. Baker, J. Mol. Spectrosc. 63, 391 (1976).

Fluorodisilane

FH_5Si_2 $H_3Si–SiH_2F$ C_s

Bond	Substitution	Effective	Angle	Effective
SiSi	2.332 B		SiSiF	109.5 X
SiF		1.598 X	SiSiH(F)[a]	110.4 X

Effective parameters determined by fitting momental equations along with the assumptions: Si–H(F) = 1.477, SiH = 1.483, HSiH(F) = 110°, HSiH = 108.3°.
[a] SiSiH angle in SiH_2F groups.

[1] A. P. Cox and R. Varma, J. Chem. Phys. 44, 2619 (1966).

Nitrosyl fluoride

FNO C_s

Bond	Substitution	Angle	Substitution
NO	1.136 B	FNO	110.1 B
NF	1.512 B		

[1] K. S. Buckton, A. C. Legon and D. J. Miller, Trans. Faraday Soc. 65, 1975 (1969).
[2] R. L. Cook, J. Chem. Phys. 42, 2927 (1965).
[3] A. Guarnieri, G. Zuliani and P. G. Favero, Nuovo Cimenti 39, 76 (1965).

Nitryl Fluoride

FNO_2 C_{2v}

Bond	Effective	Angle	Effective
NF	1.467 D	ONO	136 D
NO	1.180 C		

The oxygen coordinates were substitution coordinates.

[1] A. C. Legon and D. J. Millen, J. Chem. Soc. (A), 1736 (1968).

Thiazyl fluoride

FNS NSF C_s

Bond	Effective	Angle	Effective
NS	1.448 C	NSF	116.9 C
SF	1.643 C		

[1] R. L. Cook and W. H. Kirchhoff, J. Chem. Phys. 47, 4521 (1967).
[2] W. H. Kirchhoff and E. B. Wilson, J. Amer. Chem. Soc. 85, 1726 (1963).

Fluorotrioxorhenium

FO_3Re $FReO_3$ C_{3v}

Bond	Effective	Angle	Effective
ReO	1.692 B	FReO	109.5 C
ReF	1.859 C		

[1] J. F. Lotspeich, A. Javan, and A. Englebrecht, J. Chem. Phys. **31**, 633 (1959).

Germanium difluoride

F_2Ge FGeF C_{2v}

Bond	Equilibrium	Angle	Equilibrium
GeF	1.732 A	FGeF	97.2 A

Equilibrium structure identical for three Ge isotopic species.

[1] H. Takeo and R. F. Curl, Jr., J. Mol. Spectrosc. **43**, 21 (1972).
[2] H. Takeo, R. F. Curl, Jr., and P. W. Wilson, J. Mol. Spectrosc. **38**, 464 (1971).

Fluorimide
(Difluoramine)

F_2HN C_s

Bond	Effective	Angle	Effective
NF	1.400 B	FNF	102.9 B
NH	1.026 B	HNF	99.8 B

[1] D. R. Lide, Jr., J. Chem. Phys. **38**, 456 (1963).
[2] S. Sundaram, Proc. Phys. Soc. **92**, 261 (1967).

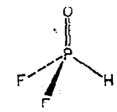
Difluorophosphine

F_2HP C_s

Bond	Effective	Angle	Effective
PF	1.582 A	FPF	99.0 A
PH	1.412 C	HPF	96.3 B

[1] R. L. Kuczkowski, J. Amer. Chem. Soc. **90**, 1705 (1968).

Difluorophosphine Oxide

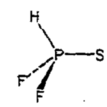


F_2HPO C_s

Bond	Effective	Angle	Effective
PH	1.387 D	HPO	117.9 D
PF	1.539 B	FPO	116.3 C
PO	1.437 B	FPF	99.8 B

[1] L. F. Centofanti and R. L. Kuczkowski, Inorg. Chem. **7**, 2582 (1968).

Hydrothiophosphoryl difluoride

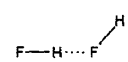


F_2HPS C_s

Bond	Effective	Angle	Effective
PH	1.392 C	SPF	117.4 B
PF	1.551 C	SPH	119.2 C
PS	1.867 C	FPF	98.6 B

[1] C. R. Nave and J. Sheridan, J. Mol. Struct. **15**, 391 (1973)

Hydrogen fluoride dimer

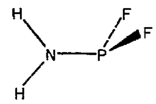


F_2H_2 C_s

Spectra consistent with bent model. With some assumptions, FF distance found to be 2.79 Å.

[1] T. R. Dyke, B. J. Howard and W. Klemperer, J. Chem. Phys. **56**, 2442 (1972).

Phosphoramidous difluoride (Aminodifluorophosphine)

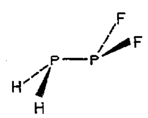


F_2H_2NP C_s

Bond	Effective	Angle	Effective
PF	1.587 B	FPF	94.6 B
PN	1.650 B	FPN	100.6 B
NH(cis)	1.002 B	PNH (cis)	123.1 B
NH (trans)	0.981 B	PNH (trans)	119.7 C
		HNH	117.2 C

[1] A. H. Brittain, J. E. Smith, P. L. Lee, K. Cohn and R. H. Schwendeman, J. Am. Chem. Soc. **93**, 6772 (1971).

Phosphinodifluorophosphine



$F_2H_2P_2$ C_s

Bond	Effective	Angle	Effective
PP	2.218 X	FPF	98.2 X
PF	1.587 X	PPF	97.2 X
		HPH	93.2 X
		PPH	90.3 X

The PH distance has been assumed to be 1.42 Å.

[1] R. L. Kuczkowski, H. W. Schiller and R. W. Rudolph, Inorg. Chem. **10**, 2505 (1971).

Krypton Difluoride

F_2Kr KrF_2 $D_{\infty h}$

Bond	Effective
KrF	1.875 D

Two possible J assignments of the ν_3 band of KrF_2 exist. The bond distance cited above is that calculated from the B_0 value from the most probable assignment. The error taken, however, is that which will encompass both possible assignments.

[1] C. Murchison, S. Reichman, D. Anderson, J. Overend and F. Schreiner, J. Am. Chem. Soc. **90**, 5690 (1968).

Difluoroamidogen (Nitrogen difluoride)

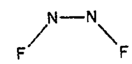
F_2N C_{2v}

Bond	Effective	Average	Angle	Effective	Average
NF	1.349 B	1.353 B	FNF	103.3 B	103.2 B

Ground state is $^2B_1$.

[1] R. D. Brown, F. R. Burden, P. D. Godfrey and J. R. Gillard, J. Mol. Spectrosc. **25**, 301 (1974).

cis–Difluorodiazine



F_2N_2 C_{2v}

Bond	Substitution	Effective	Angle	Effective
NN	1.214 B		FNN	114.6 B
NF		1.385 B		

[1] R. L. Kuczkowski and E. B. Wilson, Jr., J. Chem. Phys. **39**, 1030 (1963).

Oxygen Difluoride

F_2O C_{2v}

Bond	Effective	Average	Equilibrium
OF	1.409 A	1.412 A	1.405 A

Angle	Effective	Average	Equilibrium
FOF	103.3 A	103.2 A	103.1 A

Studies in the ground and excited states permitted determination of effective, average and equilibrium structures.

[1] L. Pierce, N. DiCianni, and R. H. Jackson, J. Chem. Phys. **38**, 730 (1963).
[2] Y. Morino and S. Saito, J. Mol. Spectrosc. **19**, 435 (1966).

Thionyl Fluoride

F_2OS		SOF_2			C_s
Bond	Effective	Average	Angle	Effective	Average
SO	1.413 A	1.416 A	FSF	92.83 A	92.79 A
SF	1.585 A	1.587 A	FSO	106.82 A	106.66 A

[1] R. C. Ferguson, J. Am. Chem. Soc. 76, 850 (1954).
[2] N. J. D. Lucas and J. G. Smith, J. Mol. Spectrosc. 43, 327 (1972).

Seleninyl Fluoride

F_2OSe		$OSeF_2$		C_s
Bond	Substitution	Effective	Angle	Effective
SeO	1.576 B		OSeF	104.8 A
SeF		1.730 A	FSeF	92.22 A

[1] I. C. Bowater, R. D. Brown, and F. R. Burden, J. Mol. Spectrosc. 28, 461 (1968).

Dioxygen Difluoride

F_2O_2		FOOF		C_2
Bond	Substitution	Effective	Angle	Effective
OO	1.217 B		OOF	109.5 B
OF		1.575 B	φ[a]	87.5 B

[a] Dihedral angle.

[1] R. H. Jackson, J. Chem. Soc. 884, 4585 (1962).

Sulfuryl Fluoride

F_2O_2S	F_2SO_2		C_{2v}
Bond	Effective	Angle	Effective
SO	1.405 C	OSO	124.0 C
SF	1.530 C	FSF	96.1 C

[1] D. R. Lide, D. E. Mann and R. M. Fristom, J. Chem. Phys. 26, 734 (1957).

Sulfur Difluoride

F_2S					C_{2v}
Bond	Effective	Average	Angle	Effective	Average
SF	1.589 G	1.592 A	FSF	98.3 B	98.2 A

[1] D. R. Johnson and F. X. Powell, Science 164, 950 (1969).
[2] W. H. Kirchhoff, D. R. Johnson, and F. X. Powell, J. Mol. Spectrosc. 48, 157 (1973).

Thionyl Fluoride

F_2SO					C_s
Bond	Effective	Average	Angle	Effective	Average
SO	1.413 B	1.416 B	FSF	92.8 B	92.8 B
SF	1.585 B	1.587 B	FSO	106.8 B	106.7 B

[1] N. J. D. Lucas and J. G. Smith, J. Mol. Spectrosc. 43, 327 (1972).
[2] R. C. Ferguson, J. Amer. Chem. Soc. 76, 850 (1954).

Disulfur Difluoride (Sulfur Monofluoride Dimer)

F_2S_2		FSSF		C_2
Bond	Substitution	Effective	Angle	Effective
SS	1.888 C		FSS	108.3 C
SF		1.635 D	φ[a]	87.9 D

[a] Dihedral angle.

[1] R. L. Kuczkowski, J. Amer. Chem. Soc. 86, 3617 (1964).

Disulfur Difluoride (Thiothionylfluoride)

F_2S_2		$S\text{-}SF_2$		C_s
Bond	Substitution	Effective	Angle	Effective
SS	1.860 D		SSF	107.5 C
SF		1.598 D	FSF	92.5 C

One sulfur atom has rather small *a* and *c* coordinates, and the second has a small *c* coordinate, which degrades the r_s S–S distance.

[1] R. L. Kuczkowski, J. Amer. Chem. Soc. 86, 3617 (1964).

Difluorosilylene (Silicon difluoride)

F_2Si — C_{2v}

Bond	Effective	Equilibrium	Angle	Effective	Equilibrium
SiF	1.591 A	1.590 A	FSiF	100.0 A	100.8 A

[1] H. Shoji, T. Tanaka and E. Hirota, J. Mol. Spectrosc. 47, 268 (1973).
[2] V. M. Rao, R. F. Curl, Jr., P. L. Timms and J. L. Margrave, J. Chem. Phys. 43, 2557 (1965).

Xenon Difluoride

F_2Xe — $D_{\infty h}$

Bond	Effective
Xe–F	1.977 B

[1] S. Reichman and F. Schreiner, J. Chem. Phys. 51, 2355 (1969).

Trifluorosilane

F_3HSi — C_{3v}

Bond	Equilibrium	Effective	Angle	Equilibrium	Effective
SiF	1.562 A	1.564 B	FSiF	108.3 A	108.3 B
SiH	1.447 A	1.455 C			

[1] A. R. Hoy, M. Bertram and I. M. Mills, J. Mol. Spectrosc. 46, 429 (1973).
[2] G. A. Heath, L. F. Thomas and J. Sheridan, Trans. Faraday Soc. 50, 779 (1954).
[3] J. Sheridan and W. Gordy, J. Chem. Phys. 19, 965 (1951).

1,1,1-Trifluorodisilane

$F_3H_3Si_2$ — $F_3Si{-}SiH_3$ — C_{3v}

Bond	Substitution	Effective	Angle	Effective
SiSi	2.319 B		SiSiH	108.7 X
SiH		1.480[a]	SiSiF	112.0 X
SiF		1.561[a]		

[a] Assumed values.

[1] J. Pasinski, S. A. McMahon and R. A. Beaudet, J. Mol. Spectrosc. 55, 88 (1975).

Trifluoroiodosilane

F_3ISi — F_3SiI — C_{3v}

Bond	Effective
SiI	2.387 D

SiF bond and FSiF angle were assumed.

[1] L. C. Sams, Jr., and A. W. Jache, J. Chem. Phys. 47, 1314 (1967).

Nitrogen Trifluoride

F_3N — C_{3v}

Bond	Effective	Equilibrium	Angle	Effective	Equilibrium
NF	1.371 A	1.365 A	FNF	102.2 A	102.4 A

[1] J. Sheridan and W. Gordy, Phys. Rev. 79, 513 (1950).
[2] M. Otake, C. Matsumura, and Y. Morino, J. Mol. Spectrosc. 28, 316 (1968).

Nitrogen Sulfur Trifluoride

F_3NS — NSF_3 — C_{3v}

Bond	Substitution	Effective	Angle	Effective
NS	1.416 C		FSF	94.0 B
SF		1.552 C		

[1] W. H. Kirchhoff and E. B. Wilson, Jr., J. Amer. Chem. Soc. 84, 334 (1962).

Phosphoryl Fluoride

F_3OP — OPF_3 — C_{3v}

Bond	Effective	Angle	Effective
PO	1.437 A	FPF	101.14 A
PF	1.522 A		

[1] R. H. Kagann, I. Ozier, and M. C. L. Gerry, Chem. Phys. Lett. 47, 572 (1977).
[2] J. G. Smith, Mol. Phys. 32, 621 (1976).

Phosphorus trifluoride

F_3P C_{3v}

Bond	Equilibrium	Average	Effective
PF	1.561 A	1.565 A	1.563 A

Angle	Equilibrium	Average	Effective
FPF	97.7 A	97.6 A	97.7 A

[1] Y. Kawashima and A. I. Cox, J. Mol. Spectrosc. **65**, 319 (1977).
[2] E. Hirota and Y. Morino, J. Mol. Spectrosc. **33**, 460 (1970).

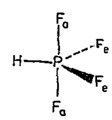
Thiophosphoryl Fluoride

F_3PS C_{3v}

Bond	Effective	Angle	Effective
PS	1.87 E	FPF	100.3 E
PF	1.53 D		

[1] Q. Williams, J. Sheridan and W. Gordy, J. Chem. Phys. **20**, 164 (1952).

Tetrafluorophosphorane



F_4HP C_{2v}

Bond	Effective	Angle	Effective
PF_a	1.596 B	HPF_a	90 E
PF_e	1.55 E	HPF_e	124 D

The PH distance was assumed.

[1] S. B. Pierce and C. D. Cornwell, J. Chem. Phys. **48**, 2118 (1968).

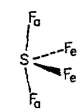
Xenon Tetrafluoride Oxide

F_4OXe $OXeF_4$ C_{4v}

Bond	Substitution	Effective	Angle	Effective
XeO	1.703 D		OXeF	91.8 C
XeF		1.900 B		

[1] J. Martins and E. B. Wilson, Jr., J. Chem. Phys. **41**, 570 (1964).
[2] J. Martins and E. B. Wilson, Jr., J. Mol. Spectrosc. **26**, 410 (1968).

Sulfur Tetrafluoride



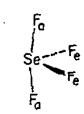
F_4S C_{2v}

Bond	Effective	Angle	Effective
SF_a	1.646 B	F_eSF_e	101.5 C
SF_e	1.545 B	F_aSF_a	186.9 C

The sulfur coordinate was a substitution coordinate.

[1] W. M. Tolles and W. D. Gwinn, J. Chem. Phys. **36**, 1119 (1962).

Selenium Tetrafluoride



F_4Se C_{2v}

Bond	Effective	Angle	Effective
SeF_a	1.771 C	F_eSeF_e	100.5 C
SeF_e	1.682 C	F_aSeF_a	169.2 C

The selenium coordinate was a substitution coordinate.

[1] I. C. Bowater, R. D. Brown, and F. R. Burden, J. Mol. Spectrosc. **28**, 454 (1968).

Iodogermane

GeH_3I $IGeH_3$ C_{3v}

Bond	Effective
GeI	2.508 B

H_3Ge projection on C_3 axis was assumed.

[1] S. N. Wolf and L. C. Krisher, J. Chem. Phys. **56**, 1040 (1972).

Germane

GeH_4 T_d

Bond	Effective
GeH	1.525 B

[1] H. W. Kattenberg, W. Gabes and A. Oskam, J. Mol. Spectrosc. 44, 425 (1972).

Germyl Silane

GeH_6Si H_3GeSiH_3 C_{3v}

Bond	Effective
GeSi	2.357 X

Parameters for the GeH_3 and SiH_3 groups were assumed.

[1] A. P. Cox and R. Varma, J. Chem. Phys. 46, 1603 (1967).

Iodosilylene

HISi HSiI C_s

Bond	Effective	Angle	Effective
SiI	2.451 B	HSiI	102.7 C

SiH distance assumed (1.561 Å).

[1] J. Billingsley, Can. J. Phys. 50, 531 (1972).

Potassium hydroxide

HKO KOH

Bond	Effective
KO	2.212 X
OH	0.912 X

The molecule has been assumed to be linear.

[1] E. F. Pearson and M. B. Trueblood, J. Chem. Phys. 58, 826 (1973).

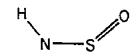
Nitrosyl Hydride

HNO C_s

Bond	Effective	Angle	Effective
NH	1.063 C	HNO	108.6 B
NO	1.212 A		

[1] F. W. Dalby, Can. J. Phys. 36, 1336 (1958).

cis-Thionylimide

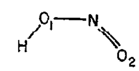


HNOS C_s

Bond	Substitution	Angle	Substitution
NH	1.029 C	HNS	115.8 C
NS	1.512 C	NSO	120.4 C
SO	1.451 C		

[1] W. H. Kirchhoff, J. Amer. Chem. Soc. 91, 2437 (1969).

cis-Nitrous Acid

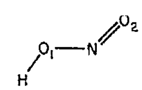


HNO_2 C_s

Bond	Effective	Angle	Effective
HO_1	0.982 D	O_1NO_2	113.6 D
NO_1	1.392 D	HO_1N	104.0 D
NO_2	1.185 D		

[1] A. P. Cox, A. H. Brittain, and D. J. Finnegan, Trans. Faraday Soc. 67, 2179 (1971).

trans-Nitrous Acid

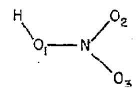


HNO_2 C_s

Bond	Substitution	Angle	Substitution
$H-O_1$	0.958 C	O_1NO_2	110.7 C
$N-O_1$	1.432 C	HO_1N	102.1 C
$N-O_2$	1.170 C		

[1] A. P. Cox, A. H. Brittain and D. J. Finnegan, Trans. Faraday Soc. 67, 2179 (1971).
[2] A. P. Cox and R. L. Kuczkowski, J. Amer. Chem. Soc. 88, 5071 (1966).

Nitric Acid

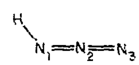


HNO_3 C_s

Bond	Substitution	Angle	Substitution
HO_1	0.964 C	HO_1N	102.2 C
NO_1	1.406 C	O_1NO_2	115.9 C
NO_2	1.211 C	O_1NO_3	113.8 C
NO_3	1.199 C	O_2NO_3	130.3 C

[1] A. P. Cox and J. M. Riveros, J. Chem. Phys. **42**, 3106 (1965).
[2] D. J. Millen and J. R. Morton, J. Chem. Soc. 1523 (1960).

Hydrazoic Acid



HN_3 C_s

Bond	Effective	Angle	Effective
N_1H	0.975 X	HN_1N_2	114.1 X
N_1N_2	1.237 X		
N_2N_3	1.133 X		

The N_3 fragment was assumed to be linear.
[1] M. Winnewisser and R. L. Cook, J. Chem. Phys. **41**, 999 (1964).

Oxophosphine

HOP HPO C_s

Bond	Effective	Angle	Effective
PO	1.512 B	HPO	104.7 C

PH distance assumed (1.433 Å).
[1] M. Lam Thanh and M. Peyron, J. Chem. Phys. **61**, 1531 (1964).

Rubidium Hydroxide

HORb RbOH

Bond	Effective	Equilibrium
RbO	2.316 C	2.301 A
OH	0.913 C	0.957 C

[1] C. Matsumura and D. R. Lide, Jr., J. Chem. Phys. **50**, 71 (196
[2] C. Matsumura and D. R. Lide, Jr., J. Chem. Phys. **50**, 3((1969).

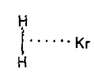
Hydroperoxyl radical

HO_2

Bond	Effective	Angle	Effective
HO	0.977 C	HOO	104.1 D
OO	1.335 C		

Ground state is $^2A''$.
[1] Y. Beers and C. J. Howard, J. Chem. Phys. **64**, 1541 (1976).
[2] J. T. Hougen, H. E. Radford, K. M. Evenson, and C. J. Howar J. Mol. Spectrosc. **56**, 210 (1975).
[3] Y. Beers and C. J. Howard, J. Chem. Phys. **63**, 4212 (1975).
[4] S. Saito, J. Mol. Spectrosc. **65**, 229 (1977).

Hydrogen Krypton(1/1)



H_2Kr Undefine

Bond	Effective
Mean value between center of mass of H_2 and Kr atom	4.07 X

[1] A. R. W. McKellar and H. L. Welsch, J. Chem. Phys. **55**, 595 (1971).

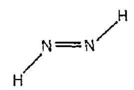
Amidogen

H_2N C_{2v}

Bond	Effective	Angle	Effective
NH	1.024 C	HNH	103.3 B

Ground electronic state is $^2B_1$.
[1] K. Dressler and D. A. Ramsay, Phil. Trans. Roy. Soc. (London) **A251**, 553 (1959).

trans-Diazine (Diimide)

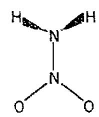


H_2N_2 C_{2h}

Distance	Effective	Angle	Effective
NH	1.028 C	HNN	106.9 C
NN	1.252 B		

[1] M. Carlotti, J. W. C. Johns and A. Trombetti, Can. J. Phys. **52**, 340 (1974).

Nitramide



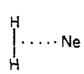
$H_2N_2O_2$ C_s

Bond	Effective	Angle	Effective
NN	1.427 X	HNH	115.2 X
NH	1.005 X	ONO	130.1 X
		φ[a]	51.8 X

[a] Angle between NH_2 and NNO_2 planes.

[1] J. K. Tyler, J. Mol. Spectrosc. **11**, 39 (1963).

Hydrogen Neon(1/1)



H_2Ne Undefined

Bond	Effective
Mean value between center of mass of H_2 and Ne atom	3.99 X

[1] A. R. W. McKellar and H. L. Welsh, Can. J. Phys. **50**, 1458 (1972).

Water

H_2O C_{2v}

Bond	Effective	Substitution	Average	Equilibrium
OH	0.965 D	0.959 C	0.972 A	0.958 A

Angle	Effective	Substitution	Average	Equilibrium
HOH	104.8 D	104.5 C	104.5 A	104.5 A

[1] R. L. Cook, F. C. DeLucia and P. Helminger, J. Mol. Spectrosc. **53**, 62 (1974).
[2] W. S. Benedict, N. Gailar, and E. K. Plyler, J. Chem. Phys. **24**, 1139 (1956).

Water(+1) Ion

H_2O^+ C_{2v}

Bond	Effective	Angle	Effective
OH	0.999 C	HOH	110.5 B

Ground electronic state is $^2B_1$.

[1] H. Lew and I. Heiber, J. Chem. Phys. **58**, 1246 (1973).

Hydrogen Peroxide

H_2O_2 C_2

Angle	Effective[a]
Dihedral	120 X

[a] Average dihedral angle in the lowest ($N = 0, \tau = 1, 2$) internal rotation states.

[1] W. C. Oelfke and W. Gordy, J. Chem. Phys. **51**, 5336 (1969).

Phosphino

H_2P C_{2v}

Bond	Effective	Angle	Effective
PH	1.418 C	HPH	91.7 B

Ground electronic state is $^2B_1$.

[1] R. N. Dixon, G. Duxbury and D. A. Ramsay, Proc. Roy. Soc. (London) **A296**, 137 (1967).
[2] J. M. Berthou, B. Pascat, H. Guenebaut and D. A. Ramsay, Can. J. Phys. **50**, 2265 (1972).

Hydrogen Sulfide

H_2S C_{2v}

Bond	Effective	Equilibrium	Angle	Effective	Substitute
HS	1.344 D	1.336 A	HSH	92.2 D	92.1 A

[1] P. Helminger, R. L. Cook and F. DeLucia, J. Chem. Phys. **56,** 4581 (1972).
[2] T. H. Edwards, N. K. Moncur and L. E. Snyder, J. Chem. Phys. **46,** 2139 (1967).

Hydrogen Sulfide(+1) Ion

H_2S^+ C_{2v}

Bond	Effective	Angle	Effective
SH	1.358 C	HSH	92.9 B

Ground electronic state is $^2B_1$.

[1] G. Duxbury, M. Horani and J. Rostas, Proc. Roy. Soc. (London) **A331,** 109 (1972).

Hydrogen Disulfide (Disulfane)

H_2S_2 HSSH C_2

Bond	Effective	Angle	Effective
SS	2.058 B	HSS	98.1 B
SH	1.345 B	Dihedral	90.8 B

Parameters were recalculated from reported data. The SD distance was assumed to be 0.003 Å shorter than the SH distance.

[1] G. Winnewisser, J. Mol. Spectrosc. **41,** 534 (1972).
[2] G. Winnewisser, M. Winnewisser, and W. Gordy, J. Chem. Phys. **49,** 3465 (1968).

Hydrogen Selenide

H_2Se

Bond	Effective	Average	Equilibrium
HSe	1.469 D	1.475 A	1.460 A

Angle	Effective	Average	Equilibrium
HSeH	90.9 D	90.6 A	90.6 A

The effective structure was calculated from the rotational cor stants of Ref. 1. The error is based on the spread in the dimensio calculated from the I_A, I_B; I_B, I_C; or I_A, I_C pairs. The average stru ture is that of Ref. 2. The equilibrium constants are those of Ref. 1 and, again the error is based on the spread in the dimensions ob tained from the various pairs of parameters. Lines from Ref. 3 wer included with infrared data in Ref. 1 to obtain the rotational con stants.

[1] R. A. Hill and T. H. Edwards, J. Chem. Phys. **42,** 1391 (1965)
[2] T. Oka and Y. Morino, J. Mol. Spectrosc. **8,** 300 (1962).
[3] A. W. Jache, P. W. Moser and W. Gordy, J. Chem. Phys. **25** 209 (1956).

Silylene

H_2Si C_{2v}

Bond	Effective	Angle	Effective
SiH	1.516 C	HSiH	92.1 B

[1] I. Dubois, Can. J. Phys. **46,** 2485 (1968).

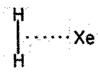
Hydrogen Telluride

H_2Te C_{2v}

Bond	Effective	Equilibrium	Angle	Effective	Equilibrium
HTe	1.653 D	1.658 B	HTeH	90.3 D	90.2 B

[1] N. K. Moncur, P. D. Willson, and T. H. Edwards, J. Mol. Spectrosc. **52,** 380 (1974).

Hydrogen–Xenon(1/1)



H_2Xe Undefined

Bond	Effective
Mean value between center of mass of H_2 and Xe atom	4.25 X

[1] A. R. W. McKellar and H. L. Welsh, J. Chem. Phys. **55**, 595 (1971).

Iodosilane

H_3ISi $ISiH_3$ C_{3v}

Bond	Substitution	Effective	Angle	Substitution	Effective
SiI	2.437 A	2.437 A	HSiI	107.8 A	108.4 B
SiH	1.485 B	1.487 B			

[1] R. Kewley, P. M. McKinney, and A. G. Robiette, J. Mol. Spectrosc. **34**, 390 (1970).
[2] A. H. Sharbaugh, G. A. Heath, L. F. Thomas, and J. Sheridan, Nature (London) **171**, 87 (1953).

Iodostannane

H_3ISn $ISnH_3$ C_{3v}

Bond	Effective
SnI	2.674 B

The projection of the SnH bond on the SnI axis was assumed.

[1] S. N. Wolf, L. C. Krisher and R. A. Gsell, J. Chem. Phys. **55**, 2106 (1971).

Ammonia

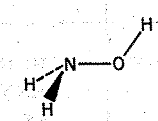
H_3N C_{3v}

Bond	Effective	Average	Substitution	Equilibrium
NH	1.017 B	1.024 B	1.014 D	1.012 B

Angle	Effective	Average	Substitution	Equilibrium
HNH	107.8 B	107.3 B	107.1 D	106.7 B

[1] W. S. Benedict and E. K. Plyler, Can. J. Phys. **35**, 1235 (1957).
[2] P. Helminger, F. C. DeLucia and W. Gordy, J. Mol. Spectrosc. **39**, 94 (1971).
[3] Y. Morino, K. Kuchitsu and S. Yamamoto, Spectrochim. Acta **24A**, 335 (1968).

Hydroxylamine



H_3NO C_s

Bond	Effective	Angle	Effective
NH	1.016 C	HNH	107.1 D
NO	1.453 B	HNO	103.2 C
OH	0.962 D	NOH	101.4 D

[1] S. Tsunekawa, J. Phys. Soc. Japan, **33**, 167 (1972).

Phosphine

H_3P PH_3 C_{3v}

Bond	Effective	Average	Angle	Effective	Average
PH	1.420 A	1.427 A	HPH	93.3 A	93.3 A

[1] F. Y. Chu and T. Oka, J. Chem. Phys. **60**, 4612 (1974).
[2] A. G. Maki, R. L. Sams and W. B. Olson, J. Chem. Phys. **58**, 4502 (1973).
[3] P. Helminger and W. Gordy, Phys. Rev. **188**, 100 (1969).

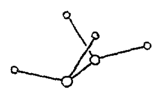
Stibine

H_3Sb — SbH_3 — C_{3v}

Bond	Substitution	Effective	Angle	Substitution	Effective
SbH	1.703 C	1.710 C	HSbH	91.5 C	91.7 C

[1] P. Helminger, E. L. Beeson, Jr., and W. Gordy, Phys. Rev. A **3**, 122(1971).
[2] A. W. Jache, G. S. Blevins, and W. Gordy, Phys. Rev. **97**, 680 (1955).

Hydrazine



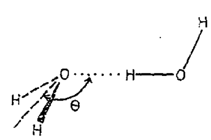
H_4N_2 — C_2

Bond	Effective	Angle	Effective
NH	1.008 D	HNH	113.3 D
NN	1.447 B	HNN	109.2 D
		ϕ^a	88.9 D

NH bonds and HNH bond angles have been assumed to be identical.
[a] Dihedral angle.

[1] S. Tsunekawa, J. Phys. Soc. Japan **41**, 2077 (1976).
[2] T. Kasuya, Sci. Pap. Inst. Phys. Chem. Res. Tokyo **56**, 1 (1962).

Water dimer



H_4O_2 — C_s

Assuming unchanged monomer geometry, the O ··· O distance is reported as 2.98 (X), and the angle θ is 58° (X).

[1] T. R. Dyke, K. M. Mack and J. S. Muenter, J. Chem. Phys. **66**, 498 (1977).

Biphosphine-4

H_4P_2 — $H^1H^2P\text{-}PH^2H^1$ — C_2

Bond	Effective	Angle	Effective
PP	2.219 B	H_1PH_2	92.0 C
PH_1	1.414 C	H_1PP	94.3 B
PH_2	1.417 C	H_2PP	99.1 B
		ϕ^a	74.0 E

[a] Dihedral angle measured from *cis* position. Hydrogens numbered H_2 are the nearly eclipsed pair.

[1] J. R. Durig, L. A. Carreira and J. D. Odom, J. Amer. Chem. Soc. **96**, 2688 (1974).

Silane

H_4Si — T_d

Bond	Effective	Substitution
SiH	1.481 A	1.479 A

[1] M. Dang-Nhu, G. Pierre and R. Saint-Loup, Mol. Phys. **28**, 447 (1974).
[2] R. W. Lovejoy and W. B. Olson, J. Chem. Phys. **57**, 2224 (1972).

Stannane

H_4Sn — T_d

Bond	Effective
SnH	1.711 B

[1] H. W. Kattenberg and A. Oskam, J. Mol. Spectrosc. **51**, 377 (1974).

Disilane

H_6Si_2 — H_3SiSiH_3 — D_{3d}

Bond	Effective	Angle	Effective
SiSi	2.327 C	HSiH	107.8 C

SiH and SiD distances were assumed.

[1] K. C. Shotton, A. G. Lee and W. J. Jones, J. Raman. Spectrosc. **1**, 243 (1973).

Nitrogen Dioxide

NO_2 C_{2v}

Bond	Substitution	Average	Angle	Substitution	Average
NO	1.197 B	1.200 B	ONO	133.8 B	133.8 B

Ground state is $^2A_1$.
Substitution values recomputed from reported rotational constants.

[1] G. R. Bird, J. C. Baird, A. W. Jache, J. A. Hodgeson, R. F. Curl, Jr., A. C. Kunkle, J. W. Bransford, J. Rastrup-Andersen, and J. Rosenthal, J. Chem. Phys. **40**, 3378 (1964).
[2] V. W. Laurie and D. R. Herschbach, J. Chem. Phys. **37**, 1687 (1962).
[3] G. R. Bird, J. Chem. Phys. **25**, 1040 (1956).

Nitrous Oxide

N_2O N=N=O $C_{\infty v}$

Bond	Equilibrium
NN	1.128 A
NO	1.184 A

[1] K. Narahari Rao, Ann. New York Acad. Sci. **220**, 17 (1973).
[2] C. A. Burrus and W. Gordy, Phys. Rev. **101**, 599 (1956).
[3] C. H. Townes and A. L. Schawlow, *Microwave Spectroscopy*, McGraw-Hill, New York (1955).

Dinitrogen Oxide(+1) Ion

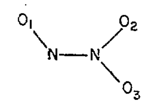
N_2O^+ NNO^+ $C_{\infty v}$

Bond	Effective
NN	1.155 C
NO	1.185 C

Ground electronic state is $^2\Pi_i$.

[1] J. H. Callomon and F. Creutzberg, Phil. Trans. Roy. Soc. **A277**, 157 (1974).

Dinitrogen trioxide



N_2O_3 C_s

Bond	Substitution	Angle	Substitution
NN	1.864 B	NNO_1	105.1 B
NO_1	1.142 C	NNO_2	112.7 B
NO_2	1.202 C	NNO_3	117.5 B
NO_3	1.217 B		

[1] A. H. Brittain, A. P. Cox and R. L. Kuczkowski, Trans. Faraday Soc. **65**, 1963 (1969).

Azido

N_3 $D_{\infty h}$

Bond	Effective
NN	1.181 A

Ground electronic state is $^2\Pi_g$.

[1] A. E. Douglas and W. J. Jones, Can. J. Phys. **43**, 2216 (1965).

Disulfur monoxide

OS_2 S_2O C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
SS	1.882 B	1.885 B	SSO	118.3 B	118.1 B
SO	1.464 B	1.462 B			

[1] E. Tiemann, J. Hoeft, F. J. Lovas and D. R. Johnson, J. Chem. Phys. **60**, 5000 (1974).
[2] D. J. Meschi and R. J. Myers, J. Mol. Spectrosc. **3**, 405 (1959).

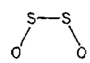
Sulfur Dioxide

O_2S SO_2 C_{2v}

Parameter	Equilibrium	Average	Substitution	Effective
SO	1.431 A	1.435 A	1.433 A	1.434 A
OSO	119.3 A	119.4 A	119.6 A	119.4 A

[1] S. Saito, J. Mol. Spectrosc. **30**, 1 (1969).
[2] Y. Morino, Y. Kikuchi, S. Saito, and E. Hirota, J. Mol. Spectrosc. **13**, 95 (1964).
[3] R. van Riet and C. Steenbeckeliers, Mém. Acad. Roy. Belg. **36**, fasc. 8 (1965).
[4] M. H. Sirvetz, J. Chem. Phys. **19**, 938 (1951).
[5] G. F. Crable and W. V. Smith, J. Chem. Phys. **19**, 502 (1951).
[6] B. P. Dailey, S. Golden, and E. B. Wilson, Phys. Rev. **72**, 871 (1947).

Sulfur monoxide dimer



O_2S_2 C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
SS	2.025 B	2.018 B	OSS	112.7 B	112.9 B
SO	1.458 B	1.469 B			

The effective parameters were calculated from reported data.

[1] F. J. Lovas, E. Tiemann and D. R. Johnson, J. Chem. Phys. **60**, 5005 (1974).

Selenium dioxide

O_2Se C_{2v}

Bond	Equilibrium	Effective	Angle	Equilibrium	Effective
SeO	1.608 A	1.609 A	OSeO	113.8 A	114.0 A

[1] E. Hirota and Y. Morino, J. Mol. Spectrosc. **34**, 370 (1970).

Ozone

O_3 C_{2v}

Bond	Equilibrium	Average	Angle	Equilibrium	Average
OO	1.272 A	1.279 A	OOO	116.8 A	116.8 A

[1] T. Tanaka and Y. Morino, J. Mol. Spectrosc. **33**, 538 (1970).
[2] R. H. Hughes, J. Chem. Phys. **24**, 131 (1956); J. Chem. Phys. **21**, 959 (1953).
[3] R. Trambarulo, S. N. Ghosh, C. A. Burrus, Jr., and W. D. Gordy, J. Chem. Phys. **21**, 851 (1953).

Sulfur Trioxide

O_3S D_{3h}

Bond	Effective
SO	1.420 A

[1] A. Kaldor and A. G. Maki, J. Mol. Struct. **15**, 123 (1973).

C_1 Molecules

Cyanogen bromide

CBrN BrCN $C_{\infty v}$

Bond	Substitution	Equilibrium
BrC	1.789 A	1.790 B
CN	1.158 A	1.157 B

[1] C. H. Townes, A. N. Holden and F. R. Merritt, Phys. Rev. **71**, 64 (1947).
[2] S. J. Tetenbaum, Phys. Rev. **86**, 440 (1952).
[3] C. A. Burrus and W. Gordy, Phys. Rev. **101**, 599 (1956).
[4] A. G. Maki and C. T. Gott, J. Chem. Phys. **36**, 2282 (1962).

Carbonyl bromide

CBr_2O C_{2v}

Bond	Effective	Angle	Effective
CO	1.172 C	BrCBr	112.3 C
CBr	1.917 C		

[1] J. H. Carpenter, J. G. Smith, I. Thompson and D. H. Whiffen, J. C. S. Faraday Trans. **1976**, 384 (1976).

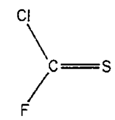
Carbonyl Chloride Fluoride

CClFO ClFCO C_s

Bond	Effective	Angle	Effective
CF	1.303 X	FCCl	112.0 X
CO	1.162 X	ClCO	117.5 X
CCl	1.751 X		

[1] A. Mirri, A. Guarneri, P. Favero, and G. Zuliani, Nuovo Cimento **25**, 265 (1962).

Chlorofluorothiocarbonyl



CClFS C_s

Bond	Average	Substitution	Effective
CCl	1.718 C	1.709 D	1.704 D
CF	1.336 C	1.347 D	1.337 D
CS	1.589 C	1.592 D	1.600 D

Angle	Average	Substitution	Effective
FCS	124.0 C	123.2 C	122.8 C
ClCS	127.6 C	127.8 C	127.7 C

Distances and angles were recalculated from reported rotational constants.

[1] R. Hamm, H. J. Kohrmann, H. Günther and W. Zeil, Z. Naturforsch. **31a**, 594 (1976).
[2] H. J. Kohrmann and W. Zeil, Z. Naturforsch. **30a**, 183 (1975).

Cyanogen Chloride

CClN ClCN $C_{\infty v}$

Bond	Equilibrium	Average	Substitution
CN	1.160 B	1.162 B	1.159 B
CCl	1.629 B	1.631 B	1.631 B

[1] W. J. Lafferty, D. R. Lide, and R. A. Toth, J. Chem. Phys. **43**, 2063 (1965).
[2] J. K. Tyler and J. Sheridan, Trans. Faraday Soc. **59**, 2661 (1963).
[3] C. H. Townes, A. N. Holden, and F. R. Merritt, Phys. Rev. **74**, 1113 (1948).
[4] A. G. Smith, H. Ring, W. V. Smith, and W. Gordy, Phys. Rev. **74**, 370 (1948).
[5] C. H. Townes, A. N. Holden, and F. R. Merritt, Phys. Rev. **71**, 64 (1947).

Chlorine Isocyanate

CClNO ClNCO C_s

Bond	Substitution	Angle	Substitution
ClN	1.705 B	ClNC	118.8 C
NC	1.226 B	NCO[a]	170.9 C
CO	1.162 B		

[a] Cl and O are trans.

[1] W. H. Hocking and M. C. L. Gerry, J. Mol. Spectrosc. **42**, 547 (1972).
[2] W. H. Hocking, M. L. Williams and M. C. L. Gerry, J. Mol. Spectrosc. **58**, 250 (1975).

Dichlorodifluoromethane

CCl_2F_2 Cl_2CF_2 C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
CCl	1.744 C		ClCCl	112.6 C	
CF		1.345 B	FCF		106.2 B

[1] H. Takeo and C. Matsumura, Bull. Chem. Soc. Japan **50**, 636 (1977).

Carbonic Dichloride
(Carbonyl chloride or phosgene)

CCl_2O $COCl_2$ C_{2v}

Bond	Effective	Angle	Effective
CO	1.166 B	ClCCl	111.3 B
CCl	1.746 B		

[1] G. Wilse Robinson, J. Chem. Phys. **21**, 1741 (1953).

Trichlorofluoromethane

CCl_3F C_{3v}

Bond	Effective	Angle	Effective
CCl	1.76 C	ClCCl	109.7 C
CF	1.33 D		

[1] M. W. Long, Q. Williams, and T. L. Weatherly, J. Chem. Phys. **33**, 508 (1960).

Cyanogen Fluoride

CFN	FCN	$C_{\infty v}$
Bond	Substitution	Effective
CF		1.262 B
CN	1.159 B	

[1] J. K. Tyler and J. Sheridan, Trans. Faraday Soc. **89**, 2661 (1963).

Difluoromethylene

CF_2 C_{2v}

Bond	Effective	Average	Angle	Effective	Average
CF	1.30 C	1.304 A	FCF	104.9 C	104.8 A

[1] W. H. Kirchhoff, D. R. Lide, and F. X. Powell, J. Mol. Spectrosc. **47**, 491 (1973).
[2] F. X. Powell and D. R. Lide, J. Chem. Phys. **45**, 1067 (1966).

(Difluoromethylene)-amidogen

CF_2N F_2CN C_{2v}

Bond	Effective	Angle	Effective
CN	1.265 D	FCF	113.5 C

Ground electronic state is $^2B_2$.
CF distance assumed (1.310 Å).

[1] R. N. Dixon, G. Duxbury, R. C. Mitchell and J. P. Simons, Proc. Roy. Soc. (London) **A300**, 405 (1967).

Phosphorocyanidous Difluoride

CF_2NP PF_2CN C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
PF	1.566 C	1.567 C	FPF	99.2 B	99.1 B
PC	1.815 B	1.811 B	FPC	96.9 B	97.1 B
CN	1.157 B	1.158 B	PCN	171.2 D	171.5 C

[1] P. L. Lee, K. Cohn, and R. H. Schwendeman, Inorg. Chem. **11**, 1917 (1972).

Difluorocyanamide

CF_2N_2 NF_2CN C_s

Bond	Effective	Substitution	Angle	Effective	Substitution
CN	1.151 B	1.158 B	NCN[a]	169.7 E	173.9 E
NC	1.392 C	1.386 C	CNF	104.7 D	105.4[b]D
NF	1.398 B	1.399[b]C	FNF	102.8 C	102.8[b]D

[a] The cyanide is tilted away from the NF_2 moiety.
[b] A mixed r_0, r_s parameter.

[1] P. L. Lee, K. Cohn and R. H. Schwendeman, Inorg. Chem. **11**, 1921 (1972).

Carbonic difluoride (Carbonyl fluoride)

CF_2O COF_2 C_{2v}

Bond	Effective	Substitution[a]	Average
CF	1.315 D	1.312[b]C	1.317 A
CO	1.170 E	1.125 C	1.170 B

Angle	Effective	Substitution[a]	Average
FCF	107.6 E	108.0[b]C	107.6 B

[a] Bond shortening correction to moments was applied prior to Kraitchman calculation.
[b] A mixed r_o, r_s parameter.

[1] D. F. Smith, M. Tidwell, D. V. P. Williams and S. J. Senatore, Phys. Rev. **83**, 485 (1951).
[2] V. W. Laurie, D. T. Pence and R. H. Jackson, J. Chem. Phys. **37**, 2995 (1962).
[3] T. Oka and Y. Morino, J. Mol. Spectrosc. **11**, 349 (1963).
[4] A. M. Mirri, F. Scappini, L. Innamorati and P. Favero, Spectrochim. Acta **25A**, 1631 (1969).
[5] J. H. Carpenter, J. Mol. Spectrosc. **50**, 182 (1974).

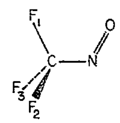
Carbonothioic Difluoride (Thiocarbonyl Fluoride)

CF_2S SCF_2 C_{2v}

Bond	Effective	Angle	Effective
CF	1.315 C	FCF	107.1 D
CS	1.589 C		

[1] A. J. Careless, H. W. Kroto and B. M. Landsberg, Chem. Phys. **1**, 371 (1973).

Trifluoronitrosomethane



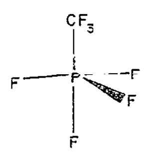
CF_3NO C_s

Bond	Effective	Angle	Effective
CF	1.324 C	F_1CN	113.9 D
NO	1.198 C	F_2CN	107.5 C
CN	1.512 D	F_2CF_3	109.8 C
		CNO	112.4 C

CF bond distances assumed equal. CF_3 group is tilted toward oxygen atom by 4.3°.

[1] P. H. Turner and A. P. Cox, Chem. Phys. Lett. **39**, 585 (1976).

Tetrafluoro(trifluoromethyl)phosphorane



CF_7P C_{3v}

CF_3 shown to be axially substituted.

[1] E. A. Cohen and C. D. Cornwell, Inorg. Chem. **7**, 398 (1968).

Tribromomethane

$CHBr_3$ $HCBr_3$ C_{3v}

Bond	Effective	Angle	Effective
CH	1.068 D	BrCBr	110.8°C
CBr	1.930 B		

[1] A. Williams, J. T. Cox and W. Gordy, J. Chem. Phys. **20**, 1524 (1952).

Chloromethylene

CHCl HCCl C_s

Bond	Effective	Angle	Effective
CH	1.12 C	HCCl	103.4 B
CCl	1.689 B		

[1] A. J. Merer and D. N. Travis, Can. J. Phys. **44**, 525 (1966).

Chlorodifluoromethane

$CHClF_2$ C_s

Bond	Substitution	Effective	Angle	Effective
CCl	1.747 D		FCCl	110.1 D
CF		1.350 D	FCF	107.0 D

CH bond and HCCl angle assumed.

[1] E. L. Beeson, T. L. Weatherly, and Q. Williams, J. Chem. Phys. **37**, 2926 (1962).
[2] D. B. McLay and C. R. Mann, Can. J. Phys. **40**, 61 (1962).

Formyl Chloride

CHClO HClCO C_s

Bond	Substitution	Angle	Substitution
CH	1.096 B	HCCl	109.9 D
CO	1.188 B	HCO	126.5 C
CCl	1.760 C		

[1] H. Takeo and C. Matsumura, J. Chem. Phys. **64**, 4536 (1976).

Dichlorofluoromethane

$CHCl_2F$ C_s

Bond	Effective	Angle	Effective
CCl	1.758 D	ClCCl	111.4 D
CF	1.346 D	ClCF	109.5 D

The parameters were calculated from the reported rotational constants. The CH distance was assumed to be 1.10 Å, and the ClCH angle was assumed equal to the FCH angle.

[1] D. B. McLay, Can. J. Phys. **42**, 720 (1964).

Chloroform

$CHCl_3$			C_{3v}
Bond	Substitution	Angle	Substitution
CCl	1.758 A	ClCCl	111.3 A
CH	1.100 B		

[1] M. Jen and D. R. Lide, J. Chem. Phys. **36**, 2525 (1962).

Fluoromethylene

CHF	HCF		C_s
Bond	Effective	Angle	Effective
CF	1.314 B	HCF	101.8 C

CH distance assumed (1.121 Å).

[1] A. J. Merer and D. N. Travis, Can. J. Phys. **44**, 1541 (1966).

Formyl Fluoride

CHFO	HFCO		C_s
Bond	Effective	Angle	Effective
CF	1.338 D	FCO	122.8 C
CO	1.181 D	HCO	127.3 D
CH	1.095 C	HCF	109.9 D

[1] R. F. Miller and R. F. Curl, Jr., J. Chem. Phys. **34**, 1847 (1961).
[2] O. H. LeBlanc, Jr., V. W. Laurie, and W. D. Gwinn, J. Chem. Phys. **33**, 598 (1960).

Trifluoromethane

CHF_3	CHF_3		C_{3v}
Bond	Effective	Angle	Effective
CH	1.098 D	FCF	108.8°C
CF	1.332 B		

[1] S. N. Ghosh, R. Trambarulo and W. Gordy. J. Chem. Phys. **20**, 605 (1952).

Hydrocyanic Acid

CHN	HCN		$C_{\infty v}$
Bond	Substitution	Effective	Equilibrium
CH	1.063 B	1.064 D	1.065 A
CN	1.155 B	1.156 D	1.153 A

[1] E. F. Pearson, R. A. Creswell, M. Winnewisser and G. Winnewisser, Z. Naturforsch. **31a**, 1394 (1976).
[2] G. Winnewisser, A. G. Maki and D. R. Johnson, J. Mol. Spectrosc. **39**, 149 (1971).
[3] F. de Lucia and W. Gordy, Phys. Rev. **187**, 58 (1969).
[4] A. G. Maki, W. B. Olson and R. L. Sams, J. Mol. Spectrosc. **36**, 433 (1970).
[5] T. Nakagawa and Y. Morino, J. Mol. Spectrosc. **31**, 208 (1969).
[6] A. G. Maki, E. K. Plyler and R. Thibault, J. Opt. Soc. Am. **54**, 869 (1964).
[7] H. C. Allen, E. D. Tidwell and E. K. Plyler, J. Chem. Phys. **25**, 302 (1956).
[8] D. H. Rank, G. Skorinko, D. P. Eastman and T. A. Wiggins, J. Opt. Soc. Am. **50**, 421 (1960).
[9] D. H. Rank, D. P. Eastman, B. S. Rao and T. A. Wiggins, J. Opt. Soc. Am. **51**, 929 (1961).
[10] W. W. Brim, J. M. Hoffman, H. H. Nielsen and K. N. Rao, J. Opt. Soc. Am. **50**, 1208 (1960).
[11] D. H. Rank, R. P. Ruth and K. L. Van der Sluis, J. Opt. Soc. Am. **42**, 693 (1952).
[12] D. H. Rank, T. A. Wiggins, A. H. Guenther and J. N. Shearer, J. Opt. Soc. Am. **46**, 953 (1956).
[13] D. H. Rank, A. H. Guenther, J. N. Shearer and T. A. Wiggins, J. Opt. Soc. Am. **47**, 148 (1957).

Isocyanic Acid

CHN	HNC	$C_{\infty v}$
Bond	Substitution	Effective
NH	0.986 B	0.986 C
CN	1.172 B	1.173 C

[1] E. F. Pearson, R. A. Creswell, M. Winnewisser and G. Winnewisser, Z. Naturforsch. **31a**, 1394 (1976).
[2] R. A. Creswell, E. F. Pearson, M. Winnewisser and G. Winnewisser, Z. Naturforsch. **31a**, 222 (1976).
[3] G. L. Blackman, R. D. Brown, P. D. Godfrey and H. I. Gunn, Nature **261**, 395 (1976).

Fulminic Acid

CHNO HCNO $C_{\infty v}$

Bond	Substitution
HC	1.027 A
NC	1.168 A
NO	1.199 A

A linear model is assumed in arriving at the substitution structure. The molecule is actually quasilinear with a large amplitude bending vibration and an equilibrium HCN angle between 155° and 170°.

[1] H. K. Bodenseh and M. F. Winnewisser, Z. Naturforsch. **24a**, 1973 (1969).
[2] B. P. Winnewisser, M. F. Winnewisser, F. Winther, J. Mol. Spectrosc. **51**, 65 (1974).

Isocyanic acid

CHNO HNCO C_s

Bond	Substitution	Angle	Substitution
NC	1.209 A	HNC	128.0 C
CO	1.166 A		
NH	0.986 D		

It was necessary to assume linearity of the NCO group. The reported values of NH and HNC are most strongly affected by this assumption, but the heavy-atom distances are also affected to a smaller extent.

[1] W. H. Hocking, M. C. L. Gerry and G. Winnewisser, Can. J. Phys. **53**, 1869 (1975).
[2] W. H. Hocking, M. C. L. Gerry and G. Winnewisser, Astrophys. J. **174**, L93 (1972).

Isothiocyanic Acid

CHNS HNCS C_s

Bond	Effective	Angle	Effective
CS	1.561 X	HNC	135.0 X
NC	1.216 X		
NH	0.989 X		

The NCS angle has been assumed to be 180°.

[1] R. Kewley, K. V. L. N. Sastry, and M. Winnewisser, J. Mol. Spectrosc. **10**, 418 (1963).
[2] C. I. Beard and B. P. Dailey, J. Chem. Phys. **18**, 1437 (1950); **19**, 975 (1951)

Cyanoamidogen

CHN_2 HNCN C_s

Bond	Effective	Angle	Effective
NH	1.034 D	HNC	116.5 E
N ··· N	2.470 A		

NCN angle assumed (180°).
Ground electronic state is $^2A''$.

[1] G. Herzberg and P. A. Warsop, Can. J. Phys. **41**, 286 (1963).

Formyl

CHO HCO C_s

Bond	Effective	Angle	Effective
CH	1.125 C	HCO	124.9 B
CO	1.175 C		

Ground state is $^2A'$.

[1] J. M. Brown and D. A. Ramsay, Can. J. Phys. **53**, 2232 (1975).
[2] J. A. Austin, D. H. Levy, C. A. Gottlieb and H. E. Radford, J. Chem. Phys. **60**, 207 (1974).
[3] S. Saito, Astrophys. J. **178**, 95 (1972).

Methylidene Phosphine

CHP HCP $C_{\infty v}$

Bond	Effective	Substitution
HC		1.068 A
CP	1.542 A	

[1] J. K. Tyler, J. Chem. Phys. **40**, 1170 (1964).

Methylene

CH_2 C_{2v}

Bond	Effective	Angle	Effective
CH	1.078 C	HCH	136 E

Ground electronic state is $^3B_1$.

[1] G. Herzberg and J. W. C. Johns, J. Chem. Phys. **54**, 2276 (1971).

Dibromomethane

CH_2Br_2 C_{2v}

Bond	Effective	Angle	Effective
CBr	1.927 C	BrCBr	112.7 B
CH	1.08 X	HCH	114 X

[1] D. Chadwick and D. J. Millen, Trans. Faraday Soc. **67**, 1539 (1971).

Chlorofluoromethane

CH_2ClF C_s

Bond	Effective	Angle	Effective
CH	1.095[a]	FCCl	109.2 X
CF	1.333 X	HCCl	109.9 X
CCl	1.797 X	HCF	109.2 X
		HCH	109.4 X

[a] This value was assumed.

[1] N. Muller, J. Am. Chem. Soc. **75**, 860 (1953).
[2] R. N. Nandi and A. Chatterji, Spectrochim. Acta **31A**, 603 (1975).

Dichloromethane

CH_2Cl_2 C_{2v}

Bond	Effective	Angle	Effective
CH	1.068 D	HCH	112.0 E
CCl	1.772 B	ClCCl	111.8 C

[1] R. J. Meyers and W. D. Gwinn, J. Chem. Phys. **20**, 1420 (1952).

Hydrogen cyanide-hydrogen fluoride dimer

CH_2FN HCN ··· HF $C_{\infty v}$

If monomer moieties are chosen as in the free monomers, NF = 2.796 (X).

[1] A. C. Legon, D. J. Millen and S. C. Rogers, Chem. Phys. Lett. **41**, 137 (1976).

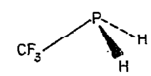
Difluoromethane

CH_2F_2 C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
CF		1.357 B	FCF		108.3 B
CH	1.093 B		HCH	113.7 B	

[1] E. Hirota and T. Tanaka, J. Mol. Spectrosc. **34**, 222 (1970).
[2] D. R. Lide, Jr., J. Amer. Chem. Soc. **74**, 3548 (1952).

(Trifluoromethyl)phosphine



CH_2F_3P C_s

Bond	Effective	Angle	Effective
CP	1.90 X	FCF	108 X
PH	1.43 X	CPH	92 X
		HPH	97 X

CF bond length was assumed.

[1] I. Yang, C. Britt, A. Cowley, and J. Boggs, J. Chem. Phys., **48**, 812 (1968).

Diazomethane

CH_2N_2 $H_2C{=}N{=}N$ C_{2v}

Bond	Substitution	Effective	Angle	Effective
NN	1.140 B		HCH	126.0 C
CN	1.300 B			
CH		1.075 C		

[1] A. P. Cox, L. F. Thomas and J. Sheridan, Nature **181**, 1000 (1958).
[2] J. Sheridan, *Advances in Molecular Spectroscopy* (Pergamon Press, Ltd., London, 1962) p. 139.
[3] C. B. Moore, J. Chem. Phys. **39**, 1884 (1963).

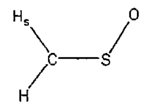
Formaldehyde

CH_2O H_2CO C_{2v}

Bond	Substitution	Average	Angle	Substitution	Average
CO	1.206 B	1.208 B	HCH	116.6 B	116.5 C
CH	1.108 B	1.116 C			

[1] K. Takagi and T. Oka, J. Phys. Soc. Japan **18**, 1174 (1963).
[2] T. Oka, J. Phys. Soc. Japan **15**, 2274 (1960).

Methanethial S-oxide (Sulfine)

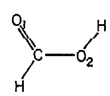


CH_2OS C_s

Bond	Substitution	Angle	Substitution
CH_s	1.085 C	HCH	121.9 C
CH	1.077 C	H_sCS	122.5 B
CS	1.610 B	HCS	115.6 C
SO	1.469 B	CSO	114.7 B

[1] R. E. Penn and R. J. Olsen, J. Mol. Spectrosc. **61**, 21 (1976).

Formic Acid



CH_2O_2 C_s

Bond	Effective	Angle	Effective
CH	1.097 X	OCO	124.6 X
CO_1	1.202 X	HCO	124.1 X
CO_2	1.343 X	COH	106.3 X
OH	0.972 X		

Numerous small coordinates lead to structure of uncertain quality.

[1] G. Kwei and R. Curl, J. Chem. Phys. **32**, 1592 (1960).
[2] A. M. Mirri, Nuovo Cimento **18**, 849 (1960).
[3] R. Lerner, J. Friend, and B. Dailey, J. Chem. Phys. **23**, 210 (1955).

Thioformaldehyde

CH_2S H_2CS C_{2v}

Bond	Substitution	Angle	Substitution
CH	1.093 C	HCH	116.9 C
CS	1.611 B		

[1] D. R. Johnson, F. X. Powell, and W. H. Kirchhoff, J. Mol. Spectrosc. **39**, 136 (1971).

Methyl

CH_3 D_{3h}

Bond	Effective
CH	1.079 B

Ground electronic state is $^2A_2''$.
The bond length is derived from B_0 of CD_3.

[1] G. Herzberg, Proc. Roy. Soc. **A262**, 291 (1961).

Carbon Monoxide–Borane (Borane carbonyl)

CH_3BO H_3BCO C_{3v}

Bond	Substitution	Effective	Angle	Substitution	Effective
BC	1.534 C	1.539 C	HBC	103.8 A	103.6 A
CO	1.135 C	1.132 C	HBH	114.5 B	114.6 B
B···O	2.669 A	2.671 B			
BH	1.222 B	1.225 B			

[1] A. C. Venkatchar, R. C. Taylor, and R. L. Kuczkowski, J. Mol. Struct. **38**, 17 (1977).
[2] W. Gordy, H. Ring, and A. B. Burg, Phys. Rev. **78**, 512 (1950).
[3] C. Pepin, L. Lambert, and A. Cabana, J. Mol. Spectrosc. **53**, 120 (1974).

Bromomethane

CH_3Br C_{3v}

Bond	Substitution	Equilibrium	Angle	Equilibrium
CBr	1.939 C	1.933 C	HCH	111.2 C
CH		1.086 C		

[1] J. L. Duncan, J. Mol. Struct. **6**, 447 (1970).
[2] R. H. Schwendeman and J. D. Kelly, J. Chem. Phys. **42**, 1132 (1965).

Bromomethylmercury

CH_3BrHg H_3CHgBr C_{3v}

Bond	Substitution	Effective	Angle	Effective
HgC	2.072 C	2.061 C	HCH	109.6° C
HgBr	2.406 C	2.405 C		
CH		1.095 C		

[1] C. Walls, D. G. Lister and J. Sheridan, J. Chem. Soc. Faraday Trans., **71**, 1091 (1975).
[2] W. Gordy and J. Sheridan, J. Chem. Phys. **22**, 92 (1954).

Choromethane

CH_3Cl C_{3v}

Bond	Substitution	Equilibrium	Angle	Equilibrium
CCl	1.781 B	1.778 B	HCH	110.7 C
CH		1.086 C		

[1] J. L. Duncan, J. Mol. Struct. **6,** 447 (1970).
[2] S. L. Miller, L. C. Aamodt, G. Dousmanis, C. H. Townes and J. Kraitchman, J. Chem. Phys. **20,** 1112 (1952).
[3] R. H. Schwendeman and J. D. Kelly, J. Chem. Phys. **42,** 1132 (1965).

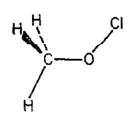
Chloromethylmercury

CH_3ClHg H_3CHgCl C_{3v}

Bond	Substitution	Effective	Angle	Effective
HgC	2.055 D	2.052 C	HCH	109.7 C
HgCl	2.283 D	2.285 C		
CH		1.092 C		

[1] C. Walls, D. G. Lister and J. Sheridan, J. Chem. Soc. Faraday Trans., **71,** 1091 (1975).
[2] J. T. Cox, T. Gäumann and W. J. Orville-Thomas, Disc. Faraday Soc. **19,** 52 (1955).
[3] W. Gordy and J. Sheridan, J. Chem. Phys. **22,** 92 (1954).

Methyl hypochlorite



CH_3ClO C_s

Bond	Effective	Angle	Effective
CH	1.101 D	COCl	110.5 D
CO	1.418 C	HCH	111.3 D
OCl	1.690 C		

The CH_3 group is tilted 5.2° away from the chlorine atom, and has been assumed to be symmetric. The parameters were recalculated from the original rotational constants.

[1] J. S. Rigden and S. S. Butcher, J. Chem. Phys. **40,** 2109 (1964).

Methanesulfenyl chloride

CH_3ClS H_3CSCl C_s

Bond	Substitution	Effective	Angle	Effective
SCl	2.030 B	2.037 B	ClSC	99.4 B
CS		1.788 B		
CH		1.082 C	θ[a]	110.2 X

Methyl group was assumed to be symmetrical, and to be staggered with respect to SCl bond.

[a] Angle between in-plane CH bond and methyl top axis.

[1] A. Guarnieri, L. Charpentier and B. Kück, Z. Naturforsch. **28a,** 1721 (1973).
[2] A. Guarnieri, Z. Naturforsch. **23a,** 1867 (1968).

Methyltrichlorogermane

CH_3Cl_3Ge H_3CGeCl_3 C_{3v}

Bond	Substitution	Angle	Substitution
GeCl	2.135 C	CGeCl	106.0 C

[1] J. R. Durig, P. J. Cooper and Y. S. Li, J. Mol. Spectrosc. **57,** 169 (1975).

Methyltrichlorosilane

CH_3Cl_3Si $H_3C\text{–}SiCl_3$ C_{3v}

Bond	Effective
SiC	1.876 X
SiCl	2.021 X

Methyl group was assumed to be tetrahedral with CH = 1.093, and angle ClSiCl was fixed at 109.4.

[1] R. C. Mockler, J. H. Bailey and W. Gordy, J. Chem. Phys. **21,** 1710 (1953).
[2] M. Mitzlaff, R. Holm and H. Hartmann, Z. Naturforsch. **22,** 1415 (1967).

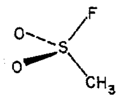
Fluoromethane

CH_3F C_{3v}

Bond	Substitution	Angle	Substitution
CF	1.383 A	HCH	110.6 B
CH	1.100 B		

[1] W. W. Clark and F. C. DeLucia, J. Mol. Struct. **32,** 29 (1976).

Methanesulfonyl Fluoride

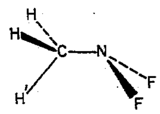


CH_3FO_2S C_s

Except for symmetry no structural results were obtained.

[1] E. J. Jacob and D. R. Lide, J. Chem. Phys. **54**, 4591 (1971).

N,N-Difluoromethylamine



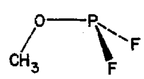
CH_3F_2N C_s

Bond	Effective	Angle	Effective
CH	1.091 C	FNF	101 E
CN	1.45 E	CNF	105 E
NF	1.41 E	NCH	110 E
		NCH′	106 E
		HCH′	112 E
		HCH	110 E

CH and CH′ assumed equal.
CH_3 and NF_2 group are staggered.

[1] L. Pierce, R. Hayes, and J. Beecher, J. Chem. Phys. **46**, 4352 (1967).

Phosphorodifluoridous acid methyl ester (Methoxydifluorophosphine)



CH_3F_2OP C_s

Bond	Effective	Angle	Effective
PF	1.591 C	FPF	94.8 D
PO	1.560 D	OPF	102.2 D
CO[a]	1.446 B	COP	123.7 C
CH	1.090 C	HCH	110.5 D

[a] This distance is r_s.

[1] E. G. Codding, C. E. Jones and R. H. Schwendeman, Inorg. Chem. **13**, 178 (1974).

Methyldifluorophosphine

CH_3F_2P CH_3PF_2 C_s

Bond	Effective	Angle	Effective
CH	1.093[a]	PCH	109.7[a]
PF	1.582[a]	FPF	98.4 C
PC	1.825 D	FPC	97.8 C

[a] Assumed values.

[1] E. G. Codding, R. A. Creswell and R. H. Schwendeman, Inorg. Chem., **13**, 856 (1974).

Methyltrifluorosilane

CH_3F_3Si H_3CSiF_3 C_{3v}

Bond	Substitution	Effective	Angle	Effective
CH	1.081 B		HCSi	111.0 B
CSi		1.812 D	FSiC	112.3 D
SiF		1.574 C		

[1] J. R. Durig, Y. S. Li, and C. C. Tong, J. Mol. Struct. **14**, 255 (1972).

Germyl Cyanide

CH_3GeN H_3GeCN C_{3v}

Bond	Substitution
GeC	1.919 B
CN	1.155 B

[1] R. Varma and K. S. Buckton, J. Chem. Phys., **46**, 1565 (1967).

Iodomethylmercury

CH_3HgI H_3CHgI C_{3v}

Bond	Substitution	Effective	Angle	Effective
HgC	2.077 C	2.069 C	HCH	109.6 C
HgI	2.571 C	2.588 C		
CH		1.095 C		

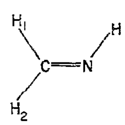
[1] C. Walls, D. G. Lister, and J. Sheridan, J. Chem. Soc., Faraday Trans., **71**, 1091 (1975).

Methyl Iodide

CH_3I			C_{3v}
Bond	Equilibrium	Angle	Equilibrium
CH	1.084 B	HCH	111.2 B
CI	2.132 B		

[1] H. Matsuura and J. Overend, J. Chem. Phys. **56**, 5725 (1972).
[2] H. Matsuura and J. Overend, Spectrochim. Acta **27A**, 2165 (1971).
[3] H. Matsuura, T. Nakagawa and J. Overend, J. Chem. Phys. **59**, 1449 (1973).
[4] R. J. L. Popplewell and H. W. Thompson, Spectrochim. Acta **25A**, 287 (1969).
[5] T. L. Barnett and T. H. Edwards, J. Mol. Spectrosc. **23**, 302 (1967).
[6] Y. Morino and C. Hirose, J. Mol. Spectrosc. **22**, 99 (1967).
[7] T. E. Sullivan and L. Frenkel, J. Mol. Spectrosc. **39**, 185 (1971).
[8] R. W. Peterson and T. H. Edwards, J. Mol. Spectrosc. **38**, 1 (1971).
[9] E. W. Jones, R. J. L. Popplewell and H. W. Thompson, Proc. Roy. Soc. **A288**, 39 (1965).
[10] J. W. Simmons and J. H. Goldstein, J. Chem. Phys. **20**, 122 (1952).

Methyleneimine

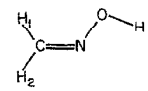


CH_3N					C_s
Bond	Substitution	Effective	Angle	Substitution	Effective
CN	1.273 C		CNH	110.5 E	
NH	1.023 D		HCH		116.9 C
CH_1		1.103 D	NCH_1		123.4 X
CH_2		1.081 D	NCH_2		119.7 X

Small *b* coordinates of C and N lead to large structural uncertainties.

[1] R. Pearson, Jr. and F. J. Lovas, J. Chem. Phys. **66**, 4149 (1977).
[2] D. R. Johnson and F. J. Lovas, Chem. Phys. Lett. **15**, 65 (1972).

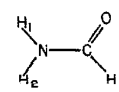
Formaldoxime



CH_3NO			C_s
Bond	Substitution	Angle	Substitution
C–N	1.276 B	H_1CN	121.8 C
NO	1.408 B	H_2CN	115.6 C
OH	0.956 B	CNO	110.2 C
CH_1	1.085 C	NOH	102.7 C
CH_2	1.086 C		

[1] I. N. Levine, J. Chem. Phys., **38**, 2326 (1963).
[2] I. N. Levine, J. Mol. Spectr., **8**, 276 (1962).

Formamide



CH_3NO			C_s
Bond	Substitution	Angle	Substitution
CN	1.352 D	H_1NH_2	121.6 C
CO	1.219 D	H_1NC	118.5 C
CH	1.098 D	NCO	124.7 C
NH_1	1.002 C	NCH	112.7 D
NH_2	1.002 C		

The molecule has been assumed to be planar, with a low-frequency single-minimum amino wagging potential function. Several small coordinates cause additional difficulties. The structure results above are a hybrid of $-NH_2$ and $-ND_2$ results.

[1] E. Hirota, R. Sugisaki, C. J. Nielsen and G. O. Sorensen, J. Mol. Spectrosc. **49**, 251 (1974).
[2] C. C. Costain and J. M. Dowling, J. Chem. Phys. **32**, 158 (1960).
[3] R. J. Kurland and E. B. Wilson, Jr., J. Chem. Phys. **27**, 585 (1957).

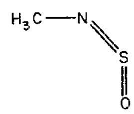
Nitrosomethane

CH_3NO $H_3C-N=O$ C_s

Isotopic substitution showed that the methyl group eclipsed the N=O bond.

[1] D. Coffey, C. O. Britt and J. E. Boggs, J. Chem. Phys. **49**, 591 (1968).

Methyl Thionylamine



CH_3NOS — C_s

Angle	Effective
CNS	122 X

Only one isotopic species was studied.

[1] V. M. Rao, J. T. Yardley, and R. F. Curl, Jr., J. Chem. Phys. **42**, 284 (1965).

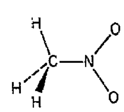
Isocyanatosilane

CH_3NOSi — $H_3SiN{=}C{=}O$ — C_{3v}

Bond	Substitution	Angle	Substitution
CO	1.179 A	HSiH	110.4 D
CN	1.150 E		
NSi	1.699 E		
SiH	1.506 C		

[1] M. C. L. Gerry, J. C. Thompson, and T. M. Sugden, Nature **211**, 846 (1966).

Nitromethane



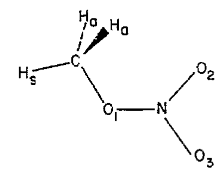
CH_3NO_2 — C_s

Bond	Substitution	Angle	Substitution
CN	1.489 B	ONO	125.3 B
NO	1.224 B	NCH	107.2 B

CH bond length was assumed (1.088 Å).

[1] A. P. Cox and S. Waring, Trans. Faraday Soc. **68**, 1060 (1972).

Methyl Nitrate



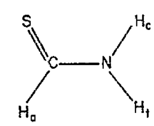
CH_3NO_3 — C_s

Bond	Substitution	Angle	Substitution
CH_a	1.095 C	H_aCH_a	109.8 C
CH_s	1.088 C	H_sCO	103.4 C
CO	1.437 B	H_aCO	110.4 C
NO_1	1.402 B	CON	112.72 B
NO_2	1.205 B	O_1NO_2	118.10 B
NO_3	1.208 B	O_2NO_3	129.52 B

Heavy atoms are coplanar. Methyl group is tilted away from O_2 by 4.8 ± 1°. Axis of NO_2 group is also tilted away from CH_3 group by 2.9°. s and a refer to in-plane and out-of-plane, respectively.

[1] A. P. Cox and S. Waring, Trans. Faraday Soc. **67**, 3441 (1971).
[2] W. B. Dixon and E. B. Wilson, J. Chem. Phys. **35**, 191 (1961).

Thioformamide



CH_3NS — C_s

Bond	Substitution	Angle	Substitution
NH_c	1.002 C	H_cNH_t	120 D
NH_t	0.99 D	H_cNC	117.9 B
CN	1.358 B	H_tNC	122 D
CS	1.626 B	NCS	125.3 B
CH_a	1.12 E	NCH_a	108 D
		SCH_a	127 D

Several parameters have been recomputed from reported data.

[1] R. Sugisaki, T. Tanaka, and E. Hirota, J. Mol. Spectrosc. **49**, 241 (1974).

Isothiocyanatosilane

CH_3NSSi	H_3SiNCS		C_{3v}
Bond	Substitution	Angle	Substitution
CN	1.211 C	HSiH	111.37 B
SiN	1.714 C		
SiH	1.489 B		

CS bond was assumed.

[1] D. R. Jenkins, R. Kewley, and T. M. Sugden, Trans. Faraday Soc. **58**, 1284 (1962).

Silanecarbonitrile

CH_3NSi	SiH_3CN		C_{3v}
Bond	Effective	Angle	Effective
SiH	1.49 E	CSiH	107.5 D
SiC	1.847 C		

CN bond was assumed.

[1] J. Sheridan and A. C. Turner, Proc. Chem. Soc. **1960**, 21 (1960).
[2] N. Muller and R. C. Bracken, J. Chem. Phys. **32**, 1577 (1960).

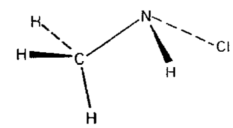
Methane

CH_4		T_d
Bond	Effective	Substitution
CH	1.094 A	1.092 A

The r_0 distance was calculated from the B_0 value of Ref. 1. The substitution distance was calculated from the data of Ref. 1 and the A_0 and B_0 reported in Ref. 2 for CH_3D.

[1] G. Tarrago, M. Dang-Nhu and G. Poussigue, J. Mol. Spectrosc. **49**, 322 (1974).
[2] W. B. Olson, J. Mol. Spectrosc. **43**, 190 (1972).

N-Chloromethylamine



CH_4ClN			C_1
Bond	Effective	Angle	Effective
CN	1.475 C	CNCl	109.4 C
NCl	1.750 C		

Deuterium substitution indicated a staggered methyl group conformation as shown in the figure.

[1] A. M. Mirri and W. Caminati, J. Mol. Spectrosc. **47**, 204 (1973).
[2] W. Caminati, R. Cervellati and A. M. Mirri, J. Mol. Spectrosc. **51**, 288 (1974).

Methyldichlorosilane

CH_4Cl_2Si	CH_3SiHCl_2		C_s
Bond	Effective	Angle	Effective
SiC	1.850[a]	SiCH	109.5[a]
SiH	1.467[a]	CSiH	110.9[a]
CH	1.093[a]	CSiCl	109.8 X
SiCl	2.040 X	ClSiCl	108.8 X

Methyl group was assumed to be symmetrical.

[a] Assumed values.

[1] K. Endo, H. Takeo and C. Matsumura, Bull. Chem. Soc. Japan **50**, 626 (1977).

Methyldifluorosilane

CH_4F_2Si	CH_3SiF_2H		C_s
Bond	Substitution	Angle	Substitution
SiC	1.840 C	FSiF	107.1 B
SiF	1.580 C	CSiH	115.53 C
SiH	1.471 C	CSiF	109.37 B
CH	1.094 B	HCH	108.53 B

Symmetrical CH_3 group assumed.

[1] L. C. Krisher and L. Pierce, J. Chem. Phys. **32**, 1619 (1960).
[2] J. D. Swalen and B. P. Stoicheff, J. Chem. Phys. **28**, 671 (1958).

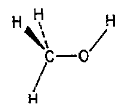
trans–Methyldiimide

CH_4N_2 CH_3NNH C_s

Insufficient data for structure determination. Only *trans* conformer found.

[1] W. Steinmetz, J. Chem. Phys. **52,** 2788 (1970).

Methanol



CH_4O C_s

Bond	Effective	Substitution	Angle	Effective	Substitution
CH	1.094 B	1.094 B	HCH	108.6 C	108.5 B
OH	0.945 B	0.963 C	COH	108.5 B	108.0 B
CO	1.425 B	1.421 A	ϕ^a	3.3 B	3.2 B

[a] Angle between CH_3 internal rotation axis and CO line; tilt is away from OH group.

[1] M. C. L. Gerry and R. M. Lees, J. Mol. Spectrosc. **61,** 231 (1976).
[2] R. M. Lees and J. G. Baker, J. Chem. Phys. **48,** 5299 (1968).
[3] Y. Y. Kwan and D. M. Dennison, J. Mol. Spectrosc. **43,** 291 (1972).

Methanethiol

CH_4S CH_3SH C_s

Bond	Effective	Angle	Effective
SH	1.335 X	CSH	96.5 X
CS	1.819 X	HCH	109.75 X
CH	1.092 X	Methyl tilt[a]	2.17 X

[a] See methanol for definition.

[1] T. Kojima, J. Phys. Soc. Japan **15,** 1284 (1960).

Methaneselenol

CH_4Se CH_3SeH C_s

Bond	Effective	Angle	Effective
SeH	1.47 X	CSeH	95.4 X
CSe	1.96 X	HCH	110.0 X
CH	1.09 X		

Internal rotation analysis indicated methyl group tilt of 1.5 ± 1.0°. See methanol for definition.

[1] C. H. Thomas, J. Chem. Phys. **59,** 70 (1974).

Chloromethylsilane

CH_5ClSi CH_2ClSiH_3 C_s

Bond	Substitution	Angle	Substitution
CSi	1.889 C	SiCCl	109.3 C
CCl	1.788 C	HSiH	110.6 C
CH	1.096 C	HCH	107.5 C
SiH	1.477 B	SiCH	109.3 C

All SiH bonds assumed equal.

[1] R. H. Schwendeman and G. D. Jacobs, J. Chem. Phys. **36,** 1251 (1962).

Methylmonofluorogermane

CH_5FGe CH_3GeH_2F C_s

Bond	Substitution	Effective	Angle	Effective
CGe	1.925 B		FGeC	106.3 D
GeF		1.751 D	HCH	108.9 C
CH		1.094 C		

GeH = 1.525Å, HGeH = 110°, and CGeH = 108.9° were assumed in order to determine GeF and FGeC. The CH_3 group was assumed to be symmetrical. There is evidence from the internal rotation that the CH_3 group is tilted 1.9° toward the F atom.

[1] R. F. Roberts, R. Varma, and J. F. Nelson, J. Chem Phys. **64,** 5035 (1976).

Methylfluorosilane

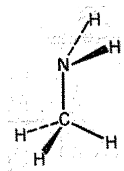
CH_5FSi CH_3SiH_2F C_s

Bond	Substitution	Angle	Substitution
SiC	1.849 B	HSiH	110.0 B
SiF	1.597 B	CSiH	112.5 D
SiH	1.477 B	HCH	108.5 B
CH	1.099 B	CSiF	108.9 B

Axial symmetry of CH_3 group was assumed.

[1] L. C. Krishner and L. Pierce, J. Chem. Phys. **32,** 1619 (1960).

Methylamine



CH_5N			C_s
Bond	Effective	Angle	Effective
CN	1.471 C	HNH	107.1 D
CH	1.099 D	HNC	110.3 D
NH	1.010 D	HCH	108.0 D
		θ[a]	3.0 C

Methyl group was assumed to be symmetrical.
[a] Angle between methyl top axis and CN bond. The methyl top axis passes through the NH_2 triangle.

[1] K. Takagi and T. Kojima, J. Phys. Soc. Japan 30, 1145 (1971).
[2] D. R. Lide, J. Chem. Phys. 27, 343 (1957).

O-Methylhydroxylamine

CH_5NO CH_3ONH_2 C_s

The *trans* conformation was established.

[1] M. Y. Fong, L. J. Johnson and M. D. Harmony, J. Mol. Spectrosc. 53, 45 (1974).

Methylphosphine

CH_5P	CH_3PH_2		C_s
Bond	Effective	Angle	Effective
CP	1.863 X	CPH	97.5 X
PH	1.414 X	HPH	93.4 X
CH	1.093 X	HCH	109.7 X
		Methyl tilt[a]	2.0 X

[a] CH_3 tilted away from PH_2 moiety.

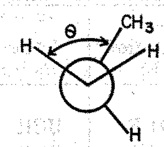
[1] T. Kojima, E. L. Breig and C. C. Lin, J. Chem. Phys. 35, 2139 (1961).

Methylgermane

CH_6Ge		CH_3GeH_3			C_{3v}
Bond	Substitution	Effective	Angle	Substitution	Effective
CH	1.083 B	1.089 B	HCH	108.4 C	108.2 C
GeH	1.529 B	1.534 B	HGeH	109.2 C	108.6 C
CGe	1.945 A				

[1] V. W. Laurie, J. Chem. Phys. 30, 1210 (1959).

Methylhydrazine

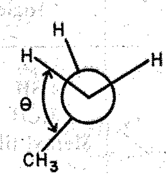


CH_6N_2	Inner Rotamer	C_1
Angle		Effective
θ		−84.5 X

Two rotamers have been observed; an inner rotamer and an outer rotamer.

[1] R. P. Lattimer and M. D. Harmony, J. Chem. Phys. 53, 4575 (1970).

Methylhydrazine



CH_6N_2	Outer Rotamer	C_1
Angle		Effective
θ		83.3 X

Two rotamers have been observed; an inner and an outer.

[1] R. P. Lattimer and M. D. Harmony, J. Chem. Phys. 53, 4575 (1970).

Methylsilane

CH_6Si		CH_3SiH_3		C_{3v}
Bond	Substitution	Effective	Angle	Effective
SiC	1.869 A		HCH	107.7 C
CH		1.093 B	HSiH	108.2 C
SiH		1.485 B		

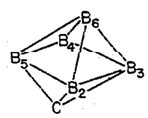
[1] R. W. Kilb and L. Pierce, J. Chem. Phys. **27**, 108 (1957).

Methylstannane

CH_6Sn	CH_3SnH_3		C_{3v}
Bond	Effective	Angle	Effective
CSn	2.143 X	HCH	109.5 X
SnH	1.700 X	HSnH	109.5 X
CH	1.09 X		

[1] D. R. Lide, Jr., J. Chem. Phys. **19**, 1605 (1951).

Monocarbahexaborane

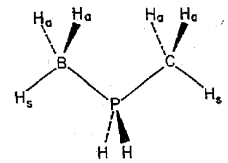


CH_7B_5	C_s
Bond	Substitution
B_2B_3	1.872 B
B_2B_6	1.888 B
B_4B_5	1.716 B
B_5B_6	1.698 B
B_2C	1.599 B
B_4C	1.633 B

The C atom and each B atom are bonded to an H atom. The seventh H atom was found to be a bridged atom in the $B_2B_3B_6$ face.

[1] G. L. McKown, B. P. Don, R. A. Beaudet, P. J. Vergamini, and L. H. Jones, J. Amer. Chem. Soc. **98**, 6909 (1976).
[2] G. L. McKown, B. P. Don, R. A. Beaudet, P. J. Vergamini, and L. H. Jones, J. Chem. Soc., Chem. Commun. **1974**, 765 (1974).

Methylphosphine-borane

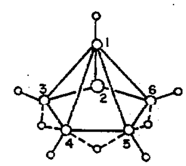


CH_8BP			C_s
Bond	Substitution	Angle	Substitution
CH_s	1.098 D	H_aBH_s	116.1 C
CH_a	1.087 B	$H_aBH_{a'}$	112.3 C
BH_a	1.229 C	H_aCH_s	110.4 D
BH_s	1.234 C	$H_aCH_{a'}$	108.1 B
PC	1.809 B	HPH′	99.9 C
PB	1.906 B	HPC	103.2 C
PH	1.404 B	CPB	115.7 B
		HPB	116.3 C
		PBH_a	102.9 C
		PBH_s	104.2 C
		PCH_a	108.3 B
		PCH_s	111.3 D

Subscripts a and s refer to out-of-plane and in-plane atoms, respectively.

[1] P. S. Bryan and R. L. Kuczkowski, Inorg. Chem. **11**, 553 (1972).

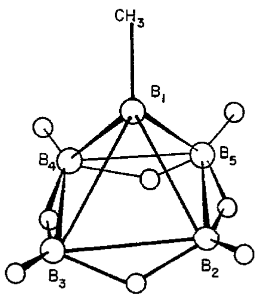
2-Carbahexaborane [(9)]



CH_7B_5			C_s
Bond	Substitution	Angle	Substitution
B_3B_4	1.759 B	$B_3B_1B_4$	59.11 C
B_4B_5	1.830 B	$B_4B_1B_5$	65.57 C
B_1B_3	1.782 B	$B_3B_4B_5$	103.9 C
B_1B_4	1.781 C		

[1] Chun-Chung S. Cheung and R. A. Beaudet, Inorg. Chem. **10**, 1144 (1971).

1-Methylpentaborane [9]



$CH_{11}B_5$		C_{4v}
Bond	Substitution	Effective
B_1B_2	1.687 C	
B_2B_3	1.800 C	
B_1C		1.62 X

[1] E. A. Cohen and R. A. Beaudet, J. Chem. Phys. **48**, 1220 (1968).

Trimethylphosphine-borane

$CH_{12}BP$ $(CH_3)_3P \cdot BH_3$ C_{3v}

Bond	Substitution	Effective	Angle	Substitution	Effective
PB		1.901 D	CPC		105.0 D
PC		1.819 D	HBH	113.5 B	
BH	1.212 C				

Methyl groups were assumed to be symmetrical and untilted, with CH = 1.080 and HCH = 109.3.

[1] P. S. Bryan and R. L. Kuczkowski, Inorg. Chem. **11**, 553 (1972).

Cyanogen iodide

CIN ICN $C_{\infty v}$

Bond	Substitution
CI	1.994 B
CN	1.159 A

[1] J. K. Tyler and J. Sheridan, Trans. Faraday Soc. **89**, 2661 (1963).

Isocyanato

CNO NCO $C_{\infty v}$

Bond	Effective
N···O	2.41 D

Ground electronic state is $^2\Pi_i$.

[1] R. N. Dixon, Phil. Trans. Roy. Soc. **A252**, 165 (1960).

Thiocyanogen

CNS NCS $C_{\infty v}$

Bond	Effective
N···S	2.82 D

Ground electronic state is $^2\Pi_i$.

[1] R. N. Dixon and D. A. Ramsay, Can. J. Phys. **46**, 2619 (1968).

Cyanoimidogen

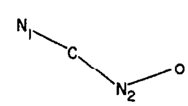
CN_2 NCN $D_{\infty h}$

Bond	Effective
CN	1.232 A

Ground electronic state is $^3\Sigma_g^-$.

[1] G. Herzberg and D. N. Travis, Can. J. Phys. **42**, 1658 (1964).

Nitrosyl cyanide



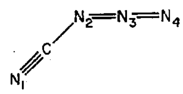
CN_2O C_s

Bond	Effective	Angle	Effective
N_1C	1.170 C	NCN	172.5 E
CN_2	1.401 C	CNO	114.7 D
NO	1.228 C		

Conclusive evidence for planarity was not presented.

[1] R. Dickinson, G. W. Kirby, J. G. Sweeny and J. K. Tyler, J. Chem. Soc. Chem. Comm. **1973**, 241 (1973).

Cyanogen Azide



CN_4 C_s

Bond	Substitution	Effective	Angle	Effective
CN_1	1.164 B		CN_2N_3[a]	120.2 D
CN_2[a]		1.312 D	N_1CN_2[a]	176 E[b]
N_2N_3[a]		1.252 D		
N_3N_4[a]		1.133 D		

[a] Derived with assumptions that $N_2N_3N_4$ linkage is linear and N_3N_4 is 1.133 ± 0.01A.

[b] N_1 bent away from N_3 linkage.

[1] K. Bolton, R. D. Brown and F. R. Burden, Chem. Phys. Lett. **15**, 79 (1972).
[2] C. C. Costain and H. W. Kroto, Can. J. Phys. **50**, 1453 (1972).
[3] G. L. Blackman, K. Bolton, R. D. Brown, F. R. Burden, and A. Mishra, J. Mol. Spectrosc. **47**, 457 (1973).

Carbonyl Sulfide

COS OCS $C_{\infty v}$

Bond	Equilibrium	Substitution
CO	1.157 A	1.160 B
CS	1.561 A	1.560 B

[1] Y. Morino and C. Matsumura, Bull. Chem. Soc. Japan **40**, 1095 (1967).
[2] C. C. Costain, J. Chem. Phys. **29**, 864 (1958).

Carbonyl Selenide

COSe OCSe $C_{\infty v}$

Bond	Substitution
CO	1.157 B
CSe	1.708 B

[1] Y. Morino and C. Matsumura, Bull. Chem. Soc. Japan **40**, 1101 (1967).

Carbon Dioxide

CO_2 OCO $D_{\infty h}$

Bond	Effective	Equilibrium
CO	1.162 A	1.160 A

[1] C. P. Courtoy, Can. J. Phys. **35**, 608 (1957).
[2] C. P. Courtoy, Ann. Soc. Sci. Brux. **73**, 5 (1959).

Carbon Dioxide(+1) Ion

CO_2^+ OCO^+ $D_{\infty h}$

Bond	Effective
CO	1.177 A

Ground electronic state is $^2\Pi_g$

[1] F. Bueso-Sanllehi, Phys. Rev. **60**, 556 (1941).
[2] S. Mrozowski, Phys. Rev. **60**, 730 (1941).
[3] S. Mrozowski, Phys. Rev. **62**, 270 (1942).
[4] S. Mrozowski, Phys. Rev. **72**, 682, 691 (1947).

Carbon Sulfide Selenide

CSSe SCSe $C_{\infty v}$

Bond	Effective
CS	1.553 A
CSe	1.695 A

[1] C. Hirose and R. F. Curl, Jr., J. Chem. Phys. **55**, 5120 (1971).

Carbon Sulfide Telluride

CSTe TeCS $C_{\infty v}$

Bond	Effective
CS	1.557 X
CTe	1.904 X

[1] W. A. Hardy and G. Silvey, Phys. Rev. **95**, 385 (1954).

Carbon Disulfide

CS_2	SCS	$D_{\infty h}$
Bond	*Effective*	*Equilibrium*
CS	1.554 A	1.553 A

[1] G. Blanquet, J. Walrand and C. P. Courtoy, Ann. Soc. Sci. Brux. **88**, 87 (1974).
[2] A. G. Maki and R. L. Sams, J. Mol. Spectrosc. **52**, 233 (1974).

Carbon Disulfide(+1) Ion

CS_2^+	SCS^+	$D_{\infty h}$
Bond		*Effective*
CS		1.554 A

Ground electronic state is $^2\Pi_g$.
[1] J. H. Callomon, Proc. Roy. Soc. **A244**, 220 (1958).

C_2 Molecules

Chloroiodoacetylene

C_2ClI	Cl—C≡C—I	$C_{\infty v}$
Bond		Effective
CC[a]		1.209
CCl		1.627 D
CI		1.989 D

[a] Assumed value.
[1] A. Bjorseth, E. Kloster-Jensen, K. M. Marstokk and H. Mollendal, J. Mol. Struct. **6**, 181 (1970).

1,1,1-Trifluoro-2,2,2-trichloroethane

$C_2Cl_3F_3$	F_3C–CCl_3		C_{3v}
Bond	Effective	Angle	Effective
CC	1.539 X	CCF	109.6 X
CF	1.330 X	CCCl	109.6 X
CCl	1.771 X		

[1] R. Holm, M. Mitzlaff and H. Hartmann, Z. Naturforsch. **23a**, 1040 (1968).

Trichloroacetonitrile

C_2Cl_3N	Cl_3CCN		C_{3v}
Bond	Effective	Angle	Effective
CCl	1.771 E	CCCl	108.9 E

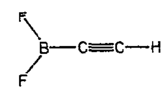
CN and CC bond lengths assumed.
[1] A. S. Rajan, Proc. Indian Acad. Sci. **53**, 89 (1961).

Trifluoroacetonitrile

C_2F_3N	CF_3CN		C_{3v}
Bond	Effective	Angle	Effective
CN	1.158[a]	FCF	108.0[a]
CF	1.335 X		
CC	1.464 X		

[a] Assumed parameters.
[1] J. Sheridan and W. Gordy, J. Chem. Phys. **20**, 591 (1952).

Ethynyldifluoroborane



C_2HBF_2			C_{2v}
Bond	Substitution	Angle	Substitution
CC	1.206 A	FBF	116.5 C
CB	1.513 B		
CH	1.058 B		
BF	1.323 C		

The fluorine parameters are not strictly substitution, since one moment of inertia relation was solved directly to obtain *x* coordinates.
[1] W. J. Lafferty and J. J. Ritter, J. Mol. Spectrosc. **38**, 181 (1971).
[2] W. J. Lafferty and J. J. Ritter, Chem. Comm. **1969**, 909 (1969).

Bromoacetylene

C_2HBr	HC≡CBr	$C_{\infty v}$
Bond	Substitution	Effective
CH		1.051 C
CC		1.216 C
CBr		1.784 C
H ··· Br	4.051 A	

[1] H. Jones, N. L. Owen, J. Sheridan, Nature **213**, 175 (1967).

Chloroacetylene

C_2HCl	$HC{\equiv}CCl$	$C_{\infty v}$

Bond	Substitution
CCl	1.637 A
CC	1.204 A
CH	1.055 A

[1] J. K. Tyler and J. Sheridan, Trans. Faraday Soc. **89**, 2661 (1963).

Fluoroacetylene

C_2HF	$HC{\equiv}CF$	$C_{\infty v}$

Bond	Substitution
CF	1.279 B
CC	1.198 B
CH	1.053 B

Authors checked C_1 coordinate by double-substitution method, since atom is close to C. of M. Agreement is well within experimental limits.

[1] J. K. Tyler and J. Sheridan, Trans. Faraday Soc. **89**, 2661 (1963).
[2] J. K. Tyler and J. Sheridan, Proc. Chem. Soc. **1960**, 119.

Iodoacetylene

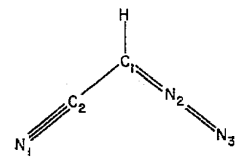
C_2HI	$HC{\equiv}CI$	$C_{\infty v}$

Bond	Effective
CI	1.988 X

In order to obtain the C—I distance it was necessary to assume both the C≡C and C—H bond distances. The unknown uncertainty in the assumptions makes it difficult to gauge the uncertainty in in the CI distance.

[1] W. Jeremy Jones, B. P. Stoicheff and J. K. Tyler, Can. J. Phys. **41**, 2098 (1963).

Diazoacetonitrile



C_2HN_3				C_s
Bond	**Substitution**	**Effective**	**Angle**	**Effective**
C_2N_1		1.165 X	$C_2C_1N_2$	119.5 X
C_2C_1		1.424 X	HC_1C_2	117 X
C_1N_2	1.280 C			
N_2N_3		1.132 X		

Linearity of $C_1N_2N_3$ was assumed. CH bond assumed.

[1] C. C. Costain and J. Yarwood, J. Chem. Phys. **45**, 1961 (1965).

Acetylene

C_2H_2	$HC{\equiv}CH$	$D_{\infty h}$

Bond	Substitution	Equilibrium
CH	1.058 B	1.061 A
CC	1.207 C	1.203 A

[1] W. J. Lafferty and R. J. Thibault, J. Mol. Spectrosc. **14**, 79 (1964).
[2] T. A. Wiggins, E. K. Plyler and E. D. Tidwell, J. Opt. Soc. Am. **51**, 1219 (1961).
[3] E. K. Plyler, E. D. Tidwell and T. A. Wiggins, J. Opt. Soc. Am. **53**, 589 (1963).
[4] W. J. Lafferty, E. K. Plyler and E. D. Tidwell, J. Chem. Phys. **37**, 1981 (1962).
[5] E. D. Tidwell and E. K. Plyler, J. Opt. Soc. Am. **52**, 656 (1962).

Bromoacetonitrile

C_2H_2BrN	$BrCH_2CN$		C_s
Bond	**Effective**	**Angle**	**Effective**
CN	1.158 X	CCBr	111.5 X
CBr	1.901 X	CCH	102.9 X
CH	1.107 X	CCN	180 X
CC	1.487 X		

[1] M. L. Gum and J. D. Graybeal, J. Mol. Spectrosc. **62**, 364 (1976).

1-Chloro-1-fluoroethylene

C_2H_2ClF $H_2C{=}CClF$ C_s

Bond	Effective	Angle	Effective
CC	1.315 X	CCH	120.0 X
CH	1.079 X	CCF	123.9 X
CF	1.325 X	CCCl	124.5 X
CCl	1.725 X		

[1] R. G. Stone and W. H. Flygare, J. Mol. Spectrosc. 32, 233 (1969).

Chloroacetonitrile

C_2H_2ClN $C^1H_2ClC^2N$ C_s

Bond	Substitution	Angle	Substitution
C^1Cl	1.781 X	C^2C^1Cl	111.5 X
C^1H	1.088 X	C^2C^1H	107.5 X

C^1C^2 and C^2N bond lengths assumed. C^1C^2 assumed linear.

[1] K. Wada, Y. Kikuchi, C. Matsumura, E. Hirota, and Y. Morino, Bull. Chem. Soc. Japan 34, 337 (1961).

1,1-Difluoroethylene

$C_2H_2F_2$ $H_2C{=}CF_2$ C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
CC		1.315 D	HCH	121.1 C	
CH	1.074 C		FCF		109.0 D
CF		1.323 D			

[1] V. W. Laurie and D. T. Pence, J. Chem. Phys. 38, 2693 (1963).

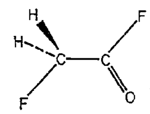
cis 1,-2-Difluoroethylene

$C_2H_2F_2$ $HFC{=}CHF$ C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
CC	1.325 A		FCC		122.1 A
CH	1.088 A		HCC	123.9 A	
CF		1.337 A			

[1] V. W. Laurie and D. T. Pence, J. Chem. Phys. 38, 2693 (1963).

trans-Fluoroacetyl fluoride



$C_2H_2F_2O$ C_s

No detailed structural information is available. A less stable (910 cal mol^{-1}) *cis* rotamer was also definitely identified.

[1] E. Saegebarth and E. B. Wilson, Jr., J. Chem. Phys. 46, 3088 (1967).

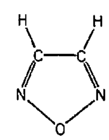
Hydrogen cyanide dimer

$C_2H_2N_2$ HCN ··· HCN $C_{\infty v}$

Assuming unchanged monomer geometry, the N ··· C distance is reported to be 3.23 Å.

[1] A. C. Legon, D. J. Millen and P. J. Mjoberg, Chem. Phys. Lett. 47, 589 (1977).

1,2,5-Oxadiazole

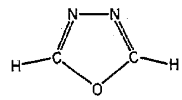


$C_2H_2N_2O$ C_{2v}

Bond	Substitution	Angle	Substitution
NO	1.380 C	NON	110.4 C
CN	1.300 B	ONC	105.8 B
CC	1.421 B	CCN	109.0 A
CH	1.076 B	CCH	130.2 A

[1] E. Saegebarth and A. P. Cox, J. Chem. Phys. 43, 166 (1965).

1,3,4-Oxadiazole

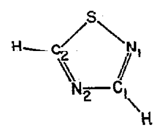


$C_2H_2N_2O$ C_{2v}

Bond	Substitution	Angle	Substitution
CO	1.348 B	COC	102.0 C
CN	1.297 C	OCN	113.4 B
NN	1.399 B	CNN	105.6 B
CH	1.075 B	OCH	118.1 B
		NCH	128.5 B

[1] L. Nygaard, R. L. Hansen, J. T. Nielsen, J. Rastrup-Andersen, G. O. Sorensen and P. A. Steiner, J. Mol. Struct. **12,** 59 (1972).

1,2,4-Thiadiazole



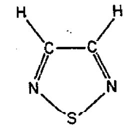
$C_2H_2N_2S$ C_s

Bond	Substitution	Angle	Substitution
SN_1	1.649 A	C_2SN_1	92.8 A
N_1C_1	1.317 A	SN_1C_1	107.1 A
C_1N_2	1.366 A	$N_1C_1N_2$	120.1 A
N_2C_2	1.313 A	$C_1N_2C_2$	107.7 A
C_2S	1.707 A	N_2C_2S	112.3 A
C_2H	1.078 B	SC_2H	123.9 B
C_1H	1.078 (Assumed)	N_2C_1H	119.9 (Assumed)

Small coordinates were present, but abundance of isotopic data yields high reliability to the structural parameters.

[1] O. L. Steifvater, Z. Naturforsch., **31a,** 1681 (1976).

1,2,5-Thiadiazole

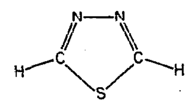


$C_2H_2N_2S$ C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
SN		1.631 B	NSN		99.5 B
NC		1.328 B	CNS		106.4 B
CC	1.418 B		CCN		113.8 B
CH		1.079 B	CCH	126.2 B	

[1] Sr. V. Dobyns and L. Pierce, J. Amer. Chem. Soc. **85,** 3553 (1963).

1,3,4-Thiadiazole

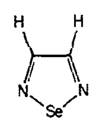


$C_2H_2N_2S$ C_{2v}

Bond	Substitution	Angle	Substitution
SC	1.721 B	CSC	86.4 A
CN	1.302 B	SCN	114.6 A
NN	1.371 B	CNN	112.2 A
CH	1.079 B	SCH	121.9 C
		NCH	123.5 C

[1] L. Nygaard, R. Lykke Hansen, and G. O. Sørensen, J. Mol. Struct. **9,** 163 (1971).
[2] B. Bak, L. Nygaard, E. J. Pedersen, and J. Rastrup-Andersen, J. Mol. Spectrosc. **19,** 283 (1966).

1,2,5-Selenadiazole

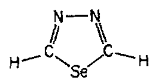


$C_2H_2N_2Se$ C_{2v}

Planar molecule with C_{2v} symmetry established.

[1] G. L. Blackman, R. D. Brown, F. R. Burden, and J. E. Kent, Chem. Phys. Lett. **1,** 379 (1967).

1,3,4-Selenadiazole

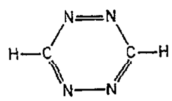


$C_2H_2N_2Se$ C_{2v}

A planar molecule with C_{2v} symmetry is definitely established.

[1] D. M. Levine, W. D. Krugh, and L. P. Gold, J. Mol. Spectrosc. **30**, 459 (1969).

s-Tetrazine



$C_2H_2N_4$ D_{2h}

Bond	Substitution	Angle	Substitution
CH	1.07 D	NCN	124.6 D
CN	1.338 D		
NN	1.330 D		

[1] A. J. Merer and K. K. Innes, Proc. Roy. Soc. (London) **A302**, 271 (1968).

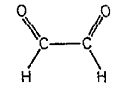
Ketene

C_2H_2O $H_2C{=}C{=}O$ C_{2v}

Bond	Substitution	Effective	Angle	Effective
CO	1.161 B		HCH	122.2 B
CC	1.314 B			
CH		1.077 B		

[1] J. W. C. Johns, J. M. R. Stone and G. Winnewisser, J. Mol. Spectrosc. **42**, 523 (1972).
[2] A. P. Cox, L. F. Thomas and J. Sheridan, Spectrochim. Acta **15**, 542 (1959).
[3] J. Sheridan, *Molecular Spectroscopy* Pergamon Press, New York 1959, pp. 139–147.
[4] H. R. Johnson and M. W. P. Strandberg, J. Chem. Phys. **20**, 687 (1952).

cis-Glyoxal



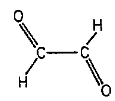
$C_2H_2O_2$ C_{2v}

Bond	Effective	Angle	Effective
CC	1.514 X	CCH	116.2 X
CH	1.130 X	CCO	123.4 D

CO distance assumed (1.207).

[1] A. R. H. Cole, Y. S. Li and J. R. Durig, J. Mol. Spectrosc. **61**, 346 (1976).
[2] D. A. Ramsey and C. Zauli, Acta Phys. Acad. Sci. Hungaricae **35**, 79 (1974).

trans-Glyoxal

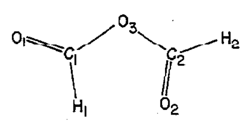


$C_2H_2O_2$ C_{2h}

Bond	Effective	Angle	Effective
CH	1.109 C	CCH	115.5 E
CC	1.527 D	CCO	121.1 A
CO	1.202 D		

[1] F. W. Birss, D. B. Braund, A. R. H. Cole, R. Engleman, Jr., A. A. Green, S. M. Japar, R. Nanes, B. J. Orr, D. A. Ramsay, and J. Szyszka, Can. J. Phys. **55**, 390 (1977).

Formic anhydride

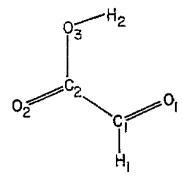


$C_2H_2O_3$ C_s

Bond	Substitution	Angle	Substitution
C_1O_1	1.184 B	$O_1C_1O_3$	120.6 B
C_1H_1	1.101 B	$H_1C_1O_3$	112.1 B
C_1O_3	1.389 B	$C_1O_3C_2$	117.8 B
C_2O_3	1.364 A	$H_2C_2O_3$	108.6 B
C_2O_2	1.195 B	$O_2C_2O_3$	126.1 B
C_2H_2	1.096 B		

[1] S. Vaccani, U. Roos, A. Bauder and Hs. H. Günthard, Chem. Phys. **19**, 51 (1977).

Glyoxylic acid

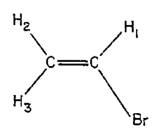


$C_2H_2O_3$ C_s

Bond	Substitution	Angle	Substitution
C_1O_1	1.174 C	$C_2C_1O_1$	123.7 C
C_2O_2	1.203 C	$C_1C_2O_2$	121.3 C
C_2O_3	1.313 D	$O_2C_2O_3$	126.2 C
C_1C_2	1.535 C	COH	107.8 B
CH	1.104 D	HCO	121.7 C
OH	0.948 B	HCC	114.6 D
		$C_1C_2O_3$	112.5 C

[1] I. Christiansen, K. M. Marstokk and H. Mollendal, J. Mol. Struct. **30**, 137 (1976).
[2] K. M. Marstokk and H. Mollendal, J. Mol. Struct. **15**, 137 (1973).

Bromoethylene (Vinyl Bromide)



C_2H_3Br C_s

Bond	Substitution	Angle	Substitution
CBr	1.904 D	CCBr	120.7 D
CC	1.334 B	CCH_1	124.3 B
CH_1	1.074 B	CCH_2	121.0 X
CH_2	1.070 X	CCH_3	121.7 B
CH_3	1.084 C		

[1] R. E. Goedertier, J. Physique **24**, 633 (1963).

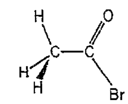
3-Methyl-3-bromodiazirine

$C_2H_3BrN_2$ $Br(CH_3)C—N{=}N$ (ring) C_s

Bond	Effective
NN	1.240 C

[1] J. E. Wollrab, J. Chem. Phys. **53**, 1543 (1970).

Acetyl bromide



C_2H_3BrO C_s

Bond	Average	Angle	Average
CO	1.181 B	OCBr	122.3 D
CBr	1.974 B	CCBr	111.0 D
CC	1.516 B	HCH	109.9 D
CH	1.092[a]	ϕ[b]	1.9 D

Methyl group has been assumed to be symmetrical.
[a] Assumed value from acetyl chloride.
[b] Methyl tilt angle; toward the oxygen.
[1] S. Tsuchiya and T. Iijima, J. Mol. Struct. **13**, 327 (1972).
[2] L. C. Krisher, J. Chem. Phys. **33**, 1237 (1970).

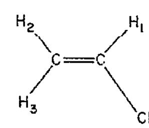
Methylbromoform

$C_2H_3Br_3$ H_3CCBr_3 C_{3v}

Bond	Effective	Angle	Effective
CBr	1.927 D	CCBr	107.7 D

Methyl group structure and CC distance were assumed from analogous molecules.
[1] Y. S. Li, K. L. Kizer and J. R. Durig, J. Mol. Spectrosc., **42**, 430 (1972).

Chloroethylene (Vinyl Chloride)



C_2H_3Cl C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
CC	1.333 B		CCCl	122.7 C	
CCl	1.726 C		CCH_1		123.0 B
CH_1		1.080 C	CCH_2		120.6 C
CH_2		1.070 C	CCH_3		121.0 C
CH_3		1.089 C			

The CCCl angle and the distances and angles involving the H atoms have been recalculated from the original data.
[1] D. Kivelson, E. B. Wilson, Jr., and D. R. Lide, Jr., J. Chem. Phys. **32**, 205 (1960).

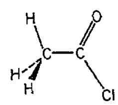
3-Methyl-3-chlorodiazirine (Methylchlorodiazirine)

$C_2H_3ClN_2$ N=N—CClCH$_3$ (ring) C_s

Bond	Effective
NN	1.241 C

[1] J. E. Wollrab and L. E. Scharpen, J. Chem. Phys. **51**, 1584 (1969).

Acetyl chloride



C_2H_3ClO C_s

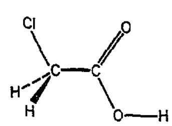
Bond	Substitution	Effective	Average
CC		1.499 D	1.505 B
CCl	1.789 B		1.796 B
CO		1.192 D	1.185 B
CH		1.083 D	1.092 B

Angle	Substitution	Effective	Average
CCO	127.1 A		127.2 B
CCCl		112.7 C	111.6 C
HCH		109.8 D	108.8 C
θ^a			1.3 C

Methyl group has been assumed to be symmetrical.
[a] Methyl group tilt angle; toward the oxygen.

[1] S. Tsuchiya and T. Iijima, J. Mol. Struct. **13**, 327 (1972).
[2] K. M. Sinnott, J. Chem. Phys. **34**, 851 (1961).

Chloroacetic acid

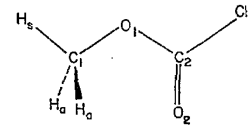


$C_2H_3ClO_2$ C_s

Only the conformation has been reliably established.

[1] B. P. Van Eijck, A. A. J. Maagdenberg and J. Wanrooy, J. Mol. Struct., **22**, 61 (1974).

Methylchloroformate



$C_2H_3ClO_2$ C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
C_2Cl		1.73 D	ClC_2O_2		126 D
C_2O_1		1.36 D	$O_1C_2O_2$		125 D
C_1O_1		1.43 D	$C_1O_1C_2$		115 D
C_1H_s	1.072 C		$O_1C_1H_s$		105 D
C_1H_a	1.076 C		$O_1C_1H_a$		110 D
			$H_aC_1H_a$	111.1 C	
			$H_sC_1H_s$	110.4 C	

The effective parameters were calculated under the assumption that the C_2O_2 bond length is 1.19 Å.

[1] J. R. Durig and M. C. Criffin, J. Mol. Spectrosc. **64**, 252 (1977).
[2] D. G. Lister and N. L. Owen, J. Chem. Soc. Faraday Trans. II **69**, 1036 (1973).

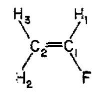
Methylchloroform

$C_2H_3Cl_3$ H_3CCCl_3 C_{3v}

Bond	Effective	Angle	Effective
CH	1.090 D	HCH	110.0 D
CC	1.541 D	CCH	108.9 D
CCl	1.771 D	ClCCl	109.4 D
		CCCl	109.6 D

[1] R. Holm, M. Mitzlaff and H. Hartmann, Z. Naturforsch. **23A**, 3071 (1968).
[2] J. R. During, M. M. Chen and Y. S. Li, J. Mol. Struct. **15**, 37 (1973).
[3] S. N. Ghosh, R. Tramburulo and W. Gordy, J. Chem. Phys. **20**, 605 (1952).
[4] W. Zeil, Z. Elektrochem. **60**, 752 (1956).

Fluoroethylene (Vinyl Fluoride)



C_2H_3F — C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
C_1C_2[a]		1.329 D	FCC		120.8 D
C_1F		1.347 D	FCH_1		110.0 E
C_1H_1		1.082 D	H_2CC[a]		120.9 D
C_2H_2	1.087 C		H_3CC[a]		119.0 D
C_2H_3	1.077 C		$H_3C_2H_2$	120.1 C	

[a] These parameters are near-substitution values. All coordinates except one coordinate of C_1 are substitution values.

[1] D. R. Lide, Jr., and D. Christensen, Spectrochim. Acta, **17**, 665 (1961).

Acetyl Fluoride

C_2H_3FO — CH_3COF — C_s

Bond	Effective	Angle	Effective
CC	1.502 B	CCF	110.7 D
CF	1.343 D	CCO	127.9 D
CO	1.185 C	CCH_i	110.4 E
CH_i	1.082 C	CCH_o	108.8 E
CH_o	1.096 C	H_iCH_i	110.8 E
		H_iCH_o	107.3 E

H_i and H_o refer to in plane and out of plane hydrogens. The oxygen atom eclipses a methyl hydrogen.

[1] L. Pierce and L. C. Krisher, J. Chem. Phys. **31**, 875 (1959).

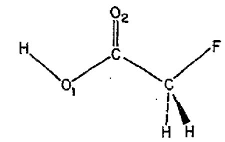
cis-Fluoroacetic acid

$C_2H_3FO_2$ — CH_2FCO_2H — C_s

cis conformer definitely established from microwave spectra, but insufficient data are available for detailed structure determination.

[1] B. P. van Eijck, G. van der Plaats and P. H. van Roon, J. Mol. Struct. **11**, 67 (1972).

trans-Fluoroacetic acid



$C_2H_3FO_2$ — C_s

Bond	Substitution
O_1H	0.973 C
O_1O_2[a]	2.258 A
O_2H[a]	2.301 C

The existence of both *cis* and *trans* forms has been definitely established from microwave spectra.

[a] These are non-bonding distances.

[1] B. P. van Eijck, C. van der Plaats and P. H. van Roon, J. Mol. Struct. **11**, 67 (1972).

1,1,2-Trifluoroethane

$C_2H_3F_3$ — $HF_2C–CH_2F$ — C_1

The stable conformation was shown to be the unsymmetrical *gauche* form.

[1] I. A. Mukhtarov, Soviet Phys. Doklady **8**, 72 (1963).
[2] I. A. Mukhtarov, Soviet Phys. Doklady **8**, 808 (1964).

Acetonitrile

C_2H_3N — CH_3CN — C_{3v}

Bond	Substitution	Angle	Substitution
CN	1.157 B	HCC	109.5 B
CC	1.458 B	DCC	109.5 B
CH	1.104 B		

[1] C. C. Costain, J. Chem. Phys., **29**, 864 (1968).
[2] C. Matsumura, E. Hirota, T. Oka, and Y. Morino, J. Mol. Spectrosc. **9**, 366 (1962).

Acetonitrile-N-oxide

C_2H_3NO — $H_3C—C≡N—O$ — C_{3v}

Bond	Substitution
CC	1.442 A
CN	1.169 B
NO	1.217 A

No data are available for H parameters.

[1] H. K. Bodenseh and K. Morgenstern, Z. Naturforsch. A **25**, 150 (1970).

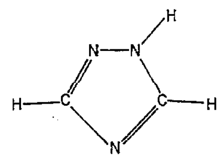
Nitroethylene

$C_2H_3NO_2$ $H_2C{=}CHNO_2$ C_s

Molecule was shown to be planar.

[1] H. Hess, A. Bander and Hs. H. Günthard, J. Mol. Spectrosc. **22**, 208 (1967).

1,2,4-Triazole



$C_2H_3N_3$ C_s

Unsymmetrical form is principal species in vapor phase. Molecule is essentially planar.

[1] K. Bolton, R. D. Brown, F. R. Burden, and A. Mishra, J. Mol. Struct. **27**, 261 (1975).
[2] K. Bolton, R. D. Brown, F. R. Burden, and A. Mishra, Chem. Commun. **1971**, 873 (1971).

Ethylene

C_2H_4 $H_2C{=}CH_2$ D_{2h}

Bond	Effective	Angle	Effective
CH	1.085 B	HCH	117.8 B
CC	1.339 B		

[1] J. L. Duncan, I. J. Wright and D. Van Lergerghe, J. Mol. Spectrosc. **42**, 463 (1972).
[2] D. Van Lerberghe, I. J. Wright and J. L. Duncan, J. Mol. Spectrosc. **42**, 251 (1972).

1-Chloro-2-fluoroethane

C_2H_4ClF $ClCH_2\text{–}CH_2F$ C_1

The observed spectrum indicated a *gauche* rotamer with a (CCF)–(CCCl) dihedral angle of 68° (X).

[1] I. A. Mukhtarov, E. S. Mukhtarov and L. A. Akhundova, J. Struct. Chem. **7**, 565 (1966).

2-Fluoroacetamide

C_2H_4FNO $FCH_2(CO)NH_2$ C_s

Microwave data showed that the heavy atom skeleton and the amino hydrogens lie in a plane, and that the C=O and C—F bonds were in the *trans* conformation.

[1] K. M. Marstokk and H. Mollendal, J. Mol. Struct. **22**, 287 (1974).

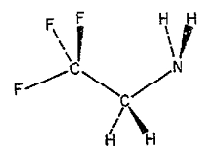
gauche 1,2-Difluoroethane

$C_2H_4F_2$ CH_2FCH_2F C_1

Dihedral angle between the two CCF planes is 73° (X).

[1] S. Butcher, R. Cohen, and T. C. Rounds, J. Chem. Phys. **54**, 4123 (1971).

trans-Trifluoroethylamine



$C_2H_4F_3N$ C_s

Molecule was shown to exist in the *trans* conformation, but detailed structure determination was not possible.

[1] I. D. Warren and E. B. Wilson, J. Chem. Phys., **56**, 2137 (1972).

Ethynylgermane (Germylacetylene)

C_2H_4Ge $H_3GeC{\equiv}CH$ C_{3v}

Bond	Substitution	Effective	Angle	Substitution	Effective
GeC	1.896 B		HGeH		109.2 X
CC	1.208 A				
GeH		1.521 X			

The CH distance has been assumed to be 1.056 Å.

[1] E. C. Thomas and V. W. Laurie, J. Chem. Phys. **44**, 2602 (1966).

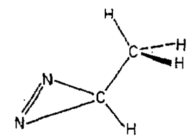
Amino acetonitrile

$C_2H_4N_2$ $H_2N\text{–}CH_2CN$ C_s

The amino group is found in the conformation in which the amino protons are *trans* to the methylene protons.

[1] H. Pickett, J. Mol. Spectrosc. **46**, 335 (1973).
[2] J. N. McDonald and J. K. Tyler, J.C.S. Chem. Comm. **1972**, 995 (1972).

3-Methyldiazirine



$C_2H_4N_2$ C_s

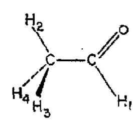
Distance	Substitution	Effective
NN		1.235 C
H_1H_2[a]	1.771 B	

The equilibrium orientation of the methyl group is staggered.

[a] Refers to non-bonding H ··· H distance in methyl group.

[1] L. H. Scharpen, J. E. Wollrab, D. P. Ames, and J. A. Merritt, J. Chem. Phys. **50**, 2063 (1969).
[2] D. W. Gord and J. E. Wollrab, J. Chem. Phys. **51**, 5728 (1969).

Acetaldehyde



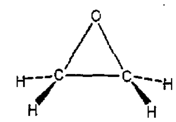
C_2H_4O C_s

Bond	Effective	Average	Angle	Effective	Average
CC	1.504 D	1.504 D	CCO	124.0 C	124.0 C
CO	1.213 D	1.217 D	CCH_1	114.9 D	
CH_1	1.106 C	1.114 D	CCH_2	110.6 C	110.2 C
CH_2	1.091 C	1.074 C	CCH_3	110.3 C	110.2 C
CH_3	1.085 C	1.074 C	H_3CH_4	108.9 C	108.7 C

The effective parameters were recalculated from reported data. The CCH_1 angle was assumed to be 117.5° and a symmetrical methyl group was assumed in the determination of the average parameters.

[1] T. Iijima and M. Kimura, Bull. Chem. Soc. Japan, **42**, 2159 (1969).
[2] R. W. Kilb, C. C. Lin, and E. B. Wilson, Jr., J. Chem. Phys. **26**, 1695 (1957).

1,2-Epoxyethane (Ethylene oxide or oxirane)



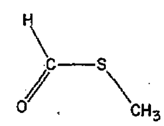
C_2H_4O C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
CC	1.466 B	1.470 B	HCH	116.6 B	116.3 B
CO	1.431 B	1.434 B	θ[a]	22.0 B	22.3 B
CH	1.085 B	1.085 B			

[a] Angle between CC bond and the line which bisects the HCH angle.

[1] C. Hirose, Bull. Chem. Soc. Japan **47**, 1311 (1974).
[2] G. L. Cunningham, A. W. Boyd, R. J. Myers and W. D. Gwinn, J. Chem. Phys. **19**, 676 (1951).

Methyl thiolformate

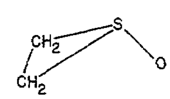


C_2H_4OS C_s

Microwave data are consistent with a *cis* conformation.

[1] G. I. L. Jones, D. G. Lister, N. L. Owen, M. C. L. Gerry and P. Palmieri, J. Mol. Spectrosc. **60**, 348 (1976).

Thiirane-1-oxide (Ethylene episulfoxide)



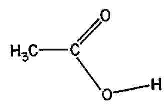
C_2H_4OS C_s

Bond	Effective	Angle	Effective
SO	1.483 D	OSC	110.0 D
CS	1.822 D	CSC	48.8 D
CC	1.504 D		

Assumptions: CH = 1.078, HCH = 116.0, HCC = 151.7.

[1] S. Saito, Bull. Chem. Soc. Japan **42**, 663 (1969).

Acetic acid

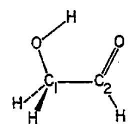


$C_2H_4O_2$ C_s

Microwave data are consistent only with the above conformation.

[1] L. C. Krisher and E. Saegebarth, J. Chem. Phys. **54**, 4553 (1971).
[2] W. J. Tabor, J. Chem. Phys. **27**, 974 (1957).

Glycolaldehyde

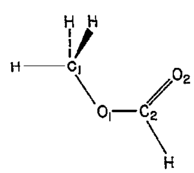


$C_2H_4O_2$ C_s

Bond	Substitution	Angle	Substitution
C_2O	1.209 A	C_1C_2O	122.7 B
C_1O	1.437 B	C_2C_1O	111.5 B
CC	1.499 A	C_1C_2H	115.3 B
OH	1.051 B	C_2C_1H	109.2 B
C_2H	1.102 B	C_1OH	101.6 B
C_1H	1.093 B	HC_1H	107.6 B

[1] K. M. Marstokk and H. Mollendal, J. Mol. Struct. **7**, 101 (1971).
[2] K. M. Marstokk and H. Mollendal, J. Mol. Struct. **16**, 259 (1973).

Methyl formate



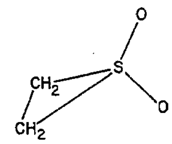
$C_2H_4O_2$ C_s

Bond	Substitution	Angle	Substitution
C_2O_2	1.200 B	$O_1C_2O_2$	125.9 B
C_2O_1	1.334 B	$C_1O_1C_2$	114.8 B
C_1O_1	1.437 B	HC_2O_1	109.3 B
C_2H	1.101 B	HC_1H	110.7 C
C_1H	1.086 C		

Methyl group has been chosen symmetrical for the reported parameters.

[1] R. F. Curl, Jr., J. Chem. Phys. **30**, 1529 (1959).

Thiirane-1,1-dioxide (Ethylene episulfone)



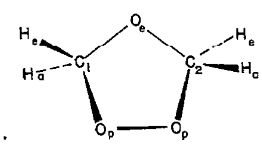
$C_2H_4O_2S$ C_{2v}

Bond	Effective	Angle	Effective
SO	1.439 D	OSO	121.4 D
CS	1.731 D	CSC	54.7 D
CC	1.590 C		

Assumptions: CH = 1.078, HCH = 116.0, HCC = 151.7.

[1] Y. Nakano, S. Saito and Y. Morino, Bull. Chem. Soc. Japan **43**, 368 (1970).

1,2,4 Trioxolane (Ethylene ozonide)

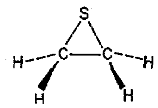


$C_2H_4O_3$ C_2

Bond	Substitution	Angle	Substitution	Dihed. Angle	Substitution
CH_e	1.091 C	COC	104.8 B	$C_1O_eC_2O_p$	−16.2 B
CH_a	1.097 C	COO	99.3 B	$C_1O_pO_pC_2$	−49.5 B
CO_e	1.416 B	OCO	105.5 B	$O_eCO_pO_p$	40.8 B
CO_p	1.412 B	HCH	113.3 C	$C_1O_eC_2H_e$	−131.3 C
O_pO_p	1.461 B	O_eCH_e	110.8 C	$C_1O_eC_2H_a$	102.8 C
		O_eCH_a	109.8 C		
		O_pCH_e	106.7 C		
		O_pCH_a	110.4 C		

[1] R. L. Kuczkowski, C. W. Gillies, and K. L. Gallaher, J. Mol. Spectrosc. **60**, 361 (1976).
[2] U. Mazur and R. L. Kuczkowski, J. Mol. Spectrosc. **65**, 84 (1977).
[3] C. W. Gillies and R. L. Kuczkowski, J. Amer. Chem. Soc. **94**, 6337 (1972).

Thiirane (Ethylene sulfide)



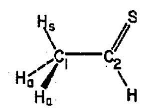
C_2H_4S C_{2v}

Bond	Substitution	Angle	Substitution
CC	1.484 B	CSC	48.3 B
CS	1.815 B	HCH	115.8 B
CH	1.083 B	ϕ^a	151.8 B

[a] Angle between HCH bisector and CC bond.

[1] K. Okiye, C. Hirose, D. G. Lister and J. Sheridan, Chem. Phys. Lett. 24, 111 (1974).
[2] G. L. Cunningham, A. W. Boyd, R. J. Myers, W. D. Gwinn and W. I. LeVan, J. Chem. Phys. 19, 676 (1951).

Thioacetaldehyde



C_2H_4S C_s

Bond	Substitution	Angle	Substitution
CS	1.610 C	CCS	125.3 C
CC	1.506 B	C_1C_2H	119.4 C
C_2H	1.089 B	$C_2C_1H_s$	111.2 C
C_1H_s	1.090 C	$C_2C_1H^a$	110.1 C
C_1H_a	1.098 D		

[1] H. W. Kroto and B. M. Landsberg, J. Mol. Spectrosc. 62, 346 (1976).

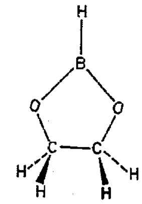
Ethynylsilane (Silyl Acetylene)

C_2H_4Si $H_3SiC{\equiv}CH$ C_{3v}

Bond	Substitution	Angle	Substitution
SiC	1.826 B	HSiH	110.2 A
CC	1.208 A		
CH	1.058 A		
SiH	1.488 A		

[1] M. C. L. Gerry and T. M. Sugden, Trans. Faraday Soc. 61, 2091 (1965).
[2] J. S. Muenter and V. W. Laurie, J. Chem. Phys. 39, 1181 (1963).

1,3,2-Dioxaborolane



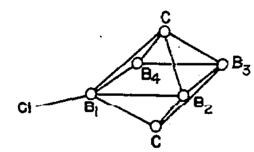
$C_2H_5BO_2$ C_2

Bond	Substitution	Effective	Angle	Substitution	Effective
CC	1.541 B		OBO		114.2 D
CO		1.438 D	BOC		107.3 D
BO		1.368 D	OCC		104.9 D
CH		1.093 D	HCH		109.2 D
BH	1.20 (assumed)		HCC		112.5 D
			α^a		11.8
			β^b		7.1

[a] α is angle between the two CCO planes.
[b] β is angle between CBC and OBO planes. HCH assumed to be bisected by OCC plane.

[1] J. H. Hund and R. H. Schwendeman, J. Chem. Phys. 45, 3349 (1966).

2-Chloro-1,6-dicarbahexaborane (6)



$C_2H_5B_4Cl$ C_{2v}

Bond	Substitution	Angle	Substitution
B_1Cl	1.823 D	$B_1B_2B_3$	87.7 C
B_1B_2	1.671 D	$B_2B_3B_4$	91.0 C
B_2B_3	1.702 C	$B_2B_1B_4$	93.6 C

In above structural drawing, each boron (except B_1) and the two carbons have one bonded hydrogen atom.

[1] G. L. McKown and R. A. Beaudet, Inorg. Chem. 10, 1350 (1971).

Bromoethane (Ethyl bromide)

C_2H_5Br — $H_3C^1\text{–}C^2H_2Br$ — C_s

Bond	Substitution	Angle	Substitution
CBr	1.950 C	CCBr	111.0 C
CC	1.518 B	C^1C^2H	112.2 C
C^1H	1.093 C	HC^2H	109.9 C
C^2H	1.087 C	HC^1H	108.9 C

Methyl group was assumed to be symmetrical.

[1] C. Flanagan and L. Pierce, J. Chem. Phys. **38**, 2963 (1963).

Chloroethane (Ethyl chloride)

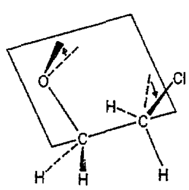
C_2H_5Cl — CH_3CH_2Cl — C_s

Bond	Substitution	Angle	Substitution
CC	1.520 B	CCCl	111.0 A
CCl	1.788 A	HCH(methyl)	108.5 C
CH(methyl)	1.091 C	HCH(methylene)	109.2 C
CH(methylene)	1.089 C	CCH(methylene)	111.6 C

Conformation is staggered. CH_3 group is assumed to be symmetrical.

[1] R. H. Schwendeman and G. D. Jacobs, J. Chem. Phys. **36**, 1245 (1962).
[2] R. S. Wagner and B. P. Dailey, J. Chem. Phys. **26**, 1588 (1957).

Chloroethanol



C_2H_5ClO — C_1

Bond	Substitution	Angle	Substitution
CCl	1.789[a]	CCCl	110.1 X
CC	1.519 X	CCO	112.8 X
CO	1.411 B	COH_1	105.8 C
OH_1	1.008 C	(CCO)–(CCCl)[b]	63.2 X
$Cl\cdots H_1$	2.609 B	$(CCO)\text{–}(COH_1)$[b]	58.4 X

[a] Assumed value.
[b] Dihedral angles between indicated planes.

[1] R. G. Azrak and E. B. Wilson, J. Chem. Phys. **52**, 5299 (1970).

Fluoroethane

C_2H_5F — CH_3CH_2F — C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
CC	1.505 B		H_gCH_g	108.9 B	
CF		1.398 B	H_gCH_t	108.7 B	
CH (methylene)	1.095 B		CCF		109.7 B
CH_g	1.090 B		HCF		106.1 B
CH_t	1.091 B		CCH (methylene)	112.9 B	
			HCH (methylene)	108.8 B	
			CCH_t	109.7 B	

Conformation is staggered. *t* and *g* refer to *trans* and *gauche* positions of methyl group protons with respect to F atom.

[1] L. Nygaard, Spectrochim. Acta **22**, 1261 (1966).
[2] B. Bak, S. Detoni, L. Hansen-Nygaard, J. T. Nielsen and J. Rastrup-Andersen, Spectrochim. Acta **16**, 376 (1960).

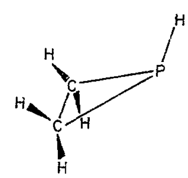
Nitroethane

$C_2H_5NO_2$ — $CH_3CH_2NO_2$ — C_s

Planarity of heavy atoms is a well-confirmed feature.

[1] Krishnaji and G. K. Panday, Indian J. Pure and App. Phys. **8**, 261 (1970).

Phosphirane



C_2H_5P — C_s

Bond	Substitution	Angle	Substitution
PC	1.867 B	HPC	95.2 B
PH	1.428 B	CCH_{cis}	118.0 B
CC	1.502 B	CCH_{trans}	117.5 B
CH_{cis}	1.092 B	HCH	114.4
CH_{trans}	1.093 B		

[1] M. T. Bowers, R. A. Beaudet, H. Goldwhite and R. Tang, J. Amer. Chem. Soc. **91**, 17 (1969).

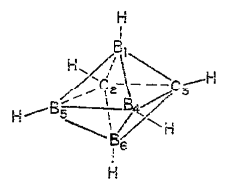
Methyl isocyanide-borane

C_2H_6BN		$C^1H_3NC^2\text{–}BH_3$	C_{3v}
Bond	Substitution	Angle	Effective
C^1N	1.416 B	HCH	110.0 C
NC^2	1.155 C	HBH	113.0 C
C^2B	1.566 B	HBC	105.7 C
		HCN	109.0 C

Effective parameters were obtained by assuming BH = 1.220 ± 0.020 and CH = 1.100 ± 0.015.

[1] J. F. Stevens, Jr., J. W. Bevan, R. F. Curl, Jr., R. A. Geanangel and M. Grace Hu, J. Amer. Chem. Soc. 99, 1442 (1977).

1,2-Dicarbahexaborane (6)



$C_2H_6B_4$			C_{2v}
Bond	Substitution	Bond	Substitution
B_1B_6	2.434 B	B_4C_3	1.605 B
C_2B_4	2.297 B	C_2C_3	1.540 B
B_1B_4	1.721 D	B_1C_2	1.627 D
B_1B_5	1.752 B		

[1] R. A. Beaudet and R. L. Poynter, J. Chem. Phys. 53, 1899 (1970).

Dimethylcadmium

C_2H_6Cd		CH_3CdCH_3	Undetermined
Bond	Effective	Angle	Effective
Cd–C	2.112 C	HCH	108.4 X

In order to obtain the HCH angle it was necessary to assume the C–H distance as 1.09 Å. The heavy atoms were assumed to be colinear.

[1] K. S. Rao, B. P. Stoicheff and R. Turner, Can. J. Phys. 38, 1516 (1960).

Vinylgermane

C_2H_6Ge		$H_2C{=}CH\text{—}GeH_3$	C_s
Bond	Effective	Angle	Effective
CC	1.347 X	CCGe	122.9 X
GeC	1.926 X	CGeH	109.7 X
GeH	1.520 X		

All vinyl hydrogen parameters have been assumed and the germyl group has been assumed to be symmetric.

[1] J. R. During, K. L. Kizer and Y. S. Li, J. Amer. Chem. Soc. 96, 7400 (1974).

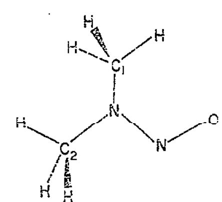
Dimethylmercury

C_2H_6Hg		CH_3HgCH_3	Undetermined
Bond	Effective	Angle	Effective
HgC	2.094 C	HCH	109.3 X

In order to obtain the HCH angle, the C–H distance was assumed. The CHgC configuration was assumed to be linear.

[1] K. S. Rao, B. P. Stoicheff and R. Turner, Can. J. Phys. 38, 1516 (1960).

N-Nitrosodimethylamine



$C_2H_6N_2O$			C_s
Bond	Effective	Angle	Effective
NN	1.329 D	NNC_1	121.4 C
NO	1.233 D	NNC_2	116.1 D
NC_1	1.444 D	NNO	114.0 C
NC_2	1.452 D	NCH[a]	111.2 X
CH[a]	1.065 X		

Although several heavy-atom isotopic species were investigated, very small coordinates yielded a structure of uncertain quality.

[a] All CH bonds and NCH angles were assumed to be identical.

[1] A. Guarnieri, F. Rohwer and F. Scappini, Z. Naturforsch. 30a, 904 (1975).
[2] F. Scappini, A. Guarnieri, H. Dreizler and P. Rademacher, Z. Naturforsch. 27a, 1329 (1972).

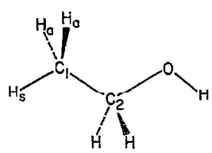
gauche-Ethanol

C_2H_6O C_1

This conformer has OH group rotated 126° (X) from the well-established *trans* position.

[1] Y. Sasada, J. Mol. Spectrosc. **38**, 33 (1971).

trans-Ethanol

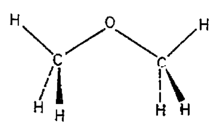


C_2H_6O C_s

Bond	Substitution	Angle	Substitution
CC	1.512 B	CCO	107.8 B
CO	1.431 B	COH	105.4 B
OH	0.971 C	C_1C_2H	110.7 B
C_2H	1.098 B	HC_2H	108.0 B
C_1H_a	1.091 C	$C_2C_1H_a$	110.1 B
C_1H_s	1.088 C	$C_2C_1H_s$	110.5 C
		$H_aC_1H_a$	108.4 B

[1] J. P. Culot, Fourth Austin Symposium on Gas Phase Molecular Structure, Paper T8 (1972).

Methyl Ether



C_2H_6O C_{2v}

Bond	Substitution	Angle	Substitution
CO	1.410 B	COC	111.7 B
CH_a	1.100 B	OCH_a	110.8 B
CH_s	1.091 C	OCH_s	107.2 C
		H_aCH_a	108.7 B
		H_aCH_s	109.5 C

Hydrogens s and a are in and out of the heavy atom plane, respectively.

[1] U. Blukis, P. H. Kasai, and R. J. Myers, J. Chem. Phys. **38**, 2753 (1963).

Methyl Sulfoxide

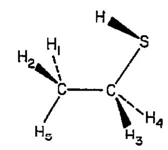
C_2H_6OS $(CH_3)_2SO$ C_s

Bond	Effective	Angle	Effective
CS	1.810 X	CSC	96.4 X
SO	1.477 X	SCH	107.5 X
CH	1.095 X	OSC	106.7 X

Methyl groups were assumed to be symmetric with C_3 axis along the CS bond.

[1] H. Dreizler and G. Dendl, Z. Naturforsch. **19a**, 512 (1964).

gauche-Ethanethiol



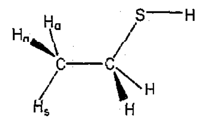
C_2H_6S C_1

Bond	Effective	Angle	Effective
SH	1.336 C	HSC	96.0 C
SC	1.814 C	CCS	113.6 C
CH_4, CH_3	1.089 D	H_4CH_3	106.6 D
CC	1.528 C	H_4CC	110.7 D
CH_5, CH_1, CH_2	1.091 D	H_3CC	111.3 D
		H_4CS	104.9 D
		H_3CS	109.3 D
		CCH_5	110.5 D
		CCH_1	110.6 D
		H_5CH_1	109.0 D
		H_1CH_2	106.9 D

Assumed: $CH_3 = CH_4$, $CH_1 = CH_2$, $CH_5 = CH_1$, and $H_5H_1 = H_5H_2$.

[1] J. Nakagawa, K. Kuwada, and M. Hayashi, Bull. Chem. Soc. Japan **49**, 3420 (1976).
[2] R. E. Schmidt and C. R. Quade, J. Chem. Phys. **62**, 864 (1975).
[3] M. Hayashi, J. Nakagawa, and K. Kuwada, Chem. Lett. **1975**, 1267 (1975).

trans-Ethanethiol



C_2H_6S			C_s
Bond	Substitution	Angle	Substitution
SH	1.322 C	CSH	96.2 B
SC	1.820 B	CCS	108.6 B
CC	1.529 B	SCH	109.4 B
CH	1.090 B	CCH	110.2 B
CH_a	1.092 C	HCH	108.9 B
CH_s	1.095 C	CCH_s	109.7 C
		CCH_a	110.6 B
		H_sCH_a	108.9 C
		H_aCH_a	108.1 C

[1] M. Hayashi, H. Imaishi, and K. Kuwada, Bull. Chem. Soc. Japan 47, 2382 (1974).
[2] M. Hayashi, H. Imaishi, K. Ohno, and H. Murata, Bull. Chem. Soc. Japan 44, 872 (1971).
[3] Ch. O. Kadzhar, A. A. Abbasov, and L. M. Imanov, Opt. Spectrosc. (USSR) 24, 334 (1968).
[4] R. E. Schmidt and C. R. Quade, Bull. Amer. Phys. Soc. II 17, 657 (1972).

Thiobismethane (Dimethyl sulfide)

C_2H_6S	CH_3SCH_3		C_{2v}
Bond	Substitution	Angle	Substitution
CS	1.802 A	CSC	98.87 A
CH_a	1.091 A	H_aCH_a	109.5 A
CH_s	1.091 E	H_aCH_s	109.6 E
		SCH_a	110.75 A
		SCH_s	106.62 E

s and a refer to methyl protons in and out of the plane of symmetry, respectively.

[1] L. Pierce and M. Hayashi, J. Chem. Phys. 35, 479 (1961).
[2] H. Dreizler and H. D. Rudolph, Z. Naturforsch. 17a, 712 (1962).

Dimethyl Disulfide

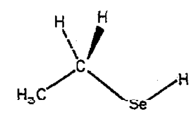
$C_2H_6S_2$	CH_3SSCH_3		C_2
Bond	Effective	Angle	Effective
SS	2.038 X	SSC	102.8 X
SC	1.810 X	SCH	108.9 X
CH	1.097 X	δ[a]	84.7 X

Methyl groups were assumed to be symmetric with C_3 axis along C–S bond.

[a] δ is the dihedral angle between the two SSC planes.

[1] D. Sutter, H. Driezler and H. D. Rudolph, Z. Naturforsch. 20a, 1676 (1965).

trans-Ethane Selenol



C_2H_6Se				C_s
Bond	Substitution	Effective	Angle	Effective
CC		1.543 C	CCSe	108.8 C
CSe		1.958 C	CSeH	93.3 C
SeH	1.444 C			

All CH parameters were assumed. A more stable *gauche* form was observed also, with a dihedral angle (measured from *cis* position) of 62.0° (X).

[1] J. R. Durig and W. E. Bucy, J. Mol. Spectrosc. 64, 474 (1977).

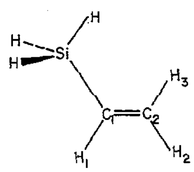
Methyl Selenide

C_2H_6Se	CH_3SeCH_3				C_{2v}
Bond	Substitution	Effective	Angle	Substitution	Effective
SeC	1.943 B		CSeC	96.2 B	
CH		1.093 C	$SeCH_a$		109.6 C
			$SeCH_s$		106.7 C
			HCH		110.3 C

Methyl groups assumed symmetric.

[1] J. F. Beecher, J. Mol. Spectrosc. 4, 414 (1966).

Vinylsilane



C_2H_6Si C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
CC	1.347 B		SiCC		122.9 C
SiC		1.853 C	HSiH		108.7 C
SiH		1.475 C	$C_2C_1H_1$	118.0 B	
C_1H_1	1.094 B		$C_1C_2H_2$		120.6 X
C_2H_3	1.097 B		$C_1C_2H_3$	120.3 B	

The C_2H_2 distance was assumed to be equal to the C_2H_3 distance. The SiH_3 group was assumed to be symmetric. The axis of the SiH_3 group is tilted 1.8° toward the methylene group.

[1] J. M. O'Reilly and L. Pierce, J. Chem. Phys. 34, 1176 (1961).

Dimethylzinc

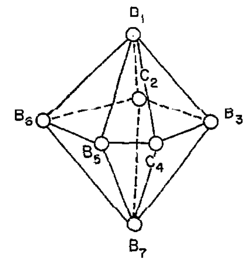
C_2H_6Zn CH_3ZnCH_3 Undetermined

Bond	Effective	Angle	Effective
C–Zn	1.929 C	HCH	107.7 X

In order to calculate the HCH angle it was necessary to assume the C–H bond distance; the uncertainty in the angle is therefore impossible to evaluate.

[1] K. S. Rao, B. P. Stoicheff and R. Turner, Can. J. Phys. 38, 1516 (1960).

2,4-Dicarbaheptaborane (7)



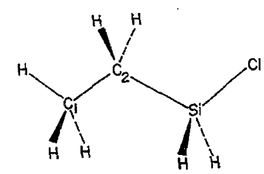
$C_2H_7B_5$ C_{2v}

Bond	Substitution	Angle	Substitution
C_2B_6	1.563 B	$C_2B_3C_4$	99.9 B
C_2B_3	1.546 B	$B_3C_4B_5$	116.8 A
C_2B_1	1.708 B	$C_4B_5B_6$	103.2 A
B_5B_6	1.651 B	$C_2B_3B_7$	79.7 C
B_1B_5	1.815 D		
B_1B_3	1.818 D		

In above figure, one hydrogen is bonded to each heavy atom.

[1] R. A. Beaudet and R. L. Poynter, J. Chem. Phys. 43, 2166 (1965).
[2] R. A. Beaudet and R. L. Poynter, J. Amer. Chem. Soc. 86, 1258 (1964).

trans-Chloroethylsilane



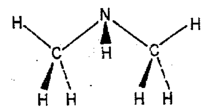
C_2H_7ClSi C_s

Bond	Effective	Angle	Effective
SiCl	2.060 X	C_2SiCl	109.9 X
SiH	1.478 X		
SiC_2	1.869 X	C_2SiH	113.6 X
C_1C_2	1.532 X	SiC_2H	105.6 X
C_2H	1.107 X	C_2C_1H	111.9 X
C_1H	1.082 X	C_1C_2Si	111.3 X
		α_1	117.7 X
		α_2	121.8 X

α_1 is the angle between the CCSi plane and the CSiH plane and α_2 is the angle between the CCSi plane and the SiCH plane. A *gauche* form exists also, with C_1C_2Si = 113.0 (X) and the SiH_2Cl group rotated by 120.4° (X).

[1] V. Typke, M. Dakkouri and W. Zeil, Z. Naturforsch. 29a, 1081 (1974).

Dimethylamine



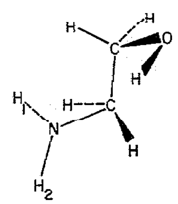
C_2H_7N C_s

Bond	Substitution	Angle	Substitution
CN	1.464 B	CNC	112.0 A
NH	1.022 C	HCH(ave)	108.5 C
CH(ave)	1.090 C	HNC	108.6 B

Within experimental error, the CH bond is found to lie in the CNC plane.

[1] J. E. Wollrab and V. W. Laurie, J. Chem. Phys. **48**, 5058 (1968).

2-Aminoethanol



C_2H_7NO C_1

Bond	Substitution	Effective	Angle	Substitution	Effective
CO		1.396 D	HNH	109.9 C	
CN		1.475 D	CCO		112.1 D
CC		1.526 D	CCN		108.1 E
OH	1.00 E		COH		108 E
NH_1	1.017 C		CNH_1		110.4 C
NH_2	1.017 C		CNH_2		111.3 C
			(OCC)–(CCN)[a]		55.4 E
			(CCO)–(COH)[a]		27 X
			(CCN)–(CNH_1)[a]		−78.2 E

OH ··· N hydrogen bond was very sensitive to isotopic substitution of D for H and, consequently, structural quality is diminished. CH parameters were assumed.

[a] Dihedral angles between indicated planes.

[1] R. E. Penn and R. F. Curl, J. Chem. Phys. **55**, 651 (1971).
[2] R. E. Penn and R. J. Olsen, J. Mol. Spectrosc. **62**, 423 (1976).

Ethylphosphine

C_2H_7P $CH_3CH_2PH_2$

Microwave data shows the presence of *trans* and *gauche* isomers, with the *trans* isomer more stable by 200 cm^{-1}.

[1] J. R. Durig and A. W. Cox, J. Chem. Phys. **64**, 1930 (1976).

Dimethylphosphine

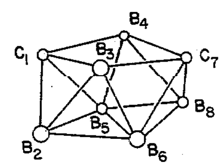
C_2H_7P $(CH_3)_2PH$ C_s

Bond	Effective	Angle	Effective
CP	1.848 X	CPC	99.7 X
PH	1.419 X	CPH	97.0 X

The methyl group was assumed to be symmetric with CH = 1.093 Å and HCH = 108.8°. The axis of the methyl group was assumed to be titled outward from the CP axis by 1°. The CH_3 group was assumed to be staggered with respect to the PH bond.

[1] R. Nelson, J. Chem. Phys. **39**, 2382 (1963).

1,7-Dicarba-*closo*-octaborane (8)



$C_2H_8B_6$ C_s

Bond	Substitution	Angle	Substitution
B_2B_3	1.813 C	$B_2B_3B_6$	52.7 B
B_2B_5	1.843 C	$B_5B_2B_6$	66.9 C
B_2B_6	1.685 C	$B_2B_6B_5$	60.4 C
B_3B_4	1.886 C	$B_2B_3B_6$	54.3 B
B_3B_6	1.880 C	$B_2B_6B_3$	60.8 B
B_5B_6	1.949 C	$B_3B_2B_6$	64.9 B

[1] H. N. Rogers, K. Lau and R. A. Beaudet, Inorg. Chem. **15**, 1775 (1976).

Dimethylgermane

C_2H_8Ge $(CH_3)_2GeH_2$ C_{2v}

Bond	Effective	Angle	Effective
GeC	1.95 C	CGeC	110 C

CH and HCH parameters assumed from CH_3GeH_3.

[1] E. C. Thomas and V. W. Laurie, J. Chem. Phys. **50**, 3512 (1969).

Ethylgermane

C_2H_8Ge	$H_3C^{(1)}C^{(2)}H_2GeH_3$		C_s
Bond	Effective	Angle	Effective
GeCl	1.949 C	GeCC	112.2 C
CC	1.545 C	HGeH	108.6 C
GeH	1.522 C	HGeC	109.7 C
$C^{(2)}H$	1.093 C	$HC^{(2)}H$	106.4 C
$C^{(1)}H$	1.091 C	$GeC^{(2)}H$	111.6 C
		$C^{(2)}C^{(1)}H$	110.9 C
		$HC^{(1)}H$	108.0 C

Methyl and germyl groups were assumed to be symmetrical.

[1] J. R. During, A. D. Lopata and P. Groner, J. Chem. Phys. **66**, 1888 (1977).

Dimethylsilane

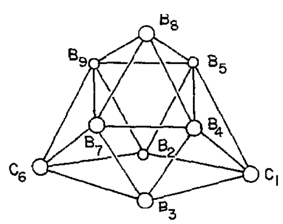
C_2H_8Si	$(CH_3)_2SiH_2$		C_{2v}
Bond	Substitution	Angle	Substitution
SiC	1.867 A	CSiC	110.98 A
SiH	1.483 B	HSiH	107.83 B
CH	1.095 B	HCH	108.00 B
		θ[a]	110.83 B

Methyl groups assumed to be symmetric.

[a] θ = angle between the symmetry axes of the two methyl groups.

[1] L. Pierce, J. Chem. Phys. **34**, 498 (1961).

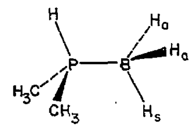
1,6-Dicarbanonaborane (9)



$C_2H_9B_7$	C_{2v}
Bond	Substitution
B_8B_9	1.712 C
B_5B_9	1.995 B
B_3B_4	1.976 C
B_7B_9	1.784 B
B_2B_3	1.805 B

[1] K. Lau and R. A. Beaudet, Inorg. Chem. **15**, 1059 (1976).

Dimethylphosphine-borane

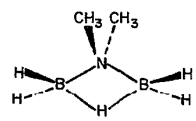


$C_2H_{10}BP$					C_s
Bond	Substitution	Effective	Angle	Substitution	Effective
BH_a	1.216 C		PBH_a	104.8 C	
BH_s	1.212 C		PBH_s	104.9 C	
PB		1.898 D	CPB		114.6 D
PC		1.813 D	CPC		105.4 D
PH		1.414 D	BPH		118.1 X

Methyl group parameters were assumed and borane group was assumed to be symmetrical about the PB bond.

[1] J. F. Durig, B. A. Hudgens, Y. S. Li and J. D. Odom, J. Chem. Phys. **61**, 4390 (1974).

μ-(Dimethylamino)diborane (6) (N,N-Dimethylaminodiborane)



$C_2H_{11}B_2N$					C_{2v}
Bond	Substitution	Effective	Angle	Substitution	Effective
BB	1.916 B		H_tBH_t	119.6 C	
BH_t	1.191 C		$BH_{br}B$	89.1 C	
BH_{br}	1.365 C		BNB[a]		76.8 X
BN[a]		1.544 X	CNC[a]		110.0 X
CN[a]		1.488 X	ϵ[b]	16.7 C	

H_t and H_{br} refer to the terminal and bridge hydrogens, respectively.

[a] Obtained by assuming methyl group parameters.

[b] Angle made by BH_2 plane and the plane perpendicular to the C_2 symmetry axis.

[1] E. A. Cohen and R. A. Beaudet, Inorg. Chem. **12**, 1570 (1973).

Bromochloroacetylene

C_2BrCl	ClC≡CBr	$C_{\infty v}$

Bond	Effective
CCl	1.628 D
CC	1.209 D
CBr	1.790 D

Ground state spectrum not observed. Rotational constants extrapolated by observing several excited vibrational states.

[1] A. Bjørseth, E. Kloster-Jensen, K. M. Marstokk, and H. Møllendal, J. Mol. Struct. 6, 181 (1970).

Isocyanomethylidyne

C_2N	CNC	$D_{\infty h}$

Bond	Effective
CN	1.245 A

Ground electronic state is $^2\Pi_g$.

[1] A. J. Merer and D. N. Travis, Can. J. Phys. 44, 353 (1966).

Cyanomethylidyne

C_2N	CCN	$C_{\infty v}$

Bond	Effective
C···N	2.56 D

Ground electronic state is $^2\Pi_r$.

[1] A. J. Merer and D. N. Travis, Can. J. Phys. 43, 1795 (1965).

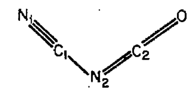
Cyanogen

C_2N_2	N≡C—C≡N	$D_{\infty h}$

Bond	Effective
CC	1.389 E
CN	1.154 D

[1] A. G. Maki, J. Chem. Phys. 43, 3193 (1965).

Cyanogen Isocyanate



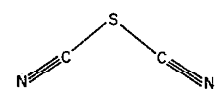
C_2N_2O			C_s

Bond	Effective	Angle	Effective
N_1C_1	1.164[a]	NCN	180[a]
N_2C_2	1.218[a]	NCO	180[a]
CO	1.165[a]	CNC	140 X
C_1N_2	1.283 X		

[a] Assumed values.

[1] W. H. Hocking and M. C. L. Gerry, J. Mol. Spectrosc. 59, 338 (1976).

Sulfur Cyanide



C_2N_2S			C_{2v}

Bond	Substitution	Angle	Substitution
SC	1.701 B	CSC	98.3 B
CN	1.156 B	SCN	175.0 C

The SCN angle is such that the angle between the two C≡N bond lines (108.3°) is larger than the CSC angle.

[1] L. Pierce, R. Nelson, and C. Thomas, J. Chem. Phys. 43, 3423 (1965).

Dicarbon Monoxide

C_2O	CCO	$C_{\infty v}$

Bond	Effective
C···O	2.52 D

Ground electronic state is $^3\Sigma^-$.

[1] C. Devillers and D. A. Ramsay, Can. J. Phys. 49, 2839 (1971).

C_3 Molecules

Tricarbon (Propadiene-1,3-diylidene)

C_3 CCC $D_{\infty h}$

Bond	Effective
CC	1.277 A

[1] A. E. Douglas, Astrophys. J. **114**, 466 (1951).
[2] L. Gausset, G. Herzberg, A. Lagerqvist and B. Rosen, Astrophys. J. **142**, 45 (1965).

Bromocyanoacetylene

C_3BrN $Br—C^1≡C^2—C^3≡N$ $C_{\infty v}$

Bond	Substitution
CBr	1.786 B
C^1C^2	1.204 B
C^2C^3	1.370 A
CN	1.159 A

[1] T. Bjorvatten, J. Mol. Struct. **20**, 75 (1974).

1-Chloro-3,3,3-Trifluoropropyne

C_3ClF_3 $F_3C^1C^2≡C^3Cl$ C_{3v}

Bond	Substitution	Effective[a]
C^3Cl	1.629 C	1.627 C
$C^1 \cdots C^3$	2.647 B	
C^1C^2		1.453 C
C^2C^3		1.199 C
C^1F		1.336 C

[a] The FCF angle was assumed in order to determine these parameters.

[1] A. Bjørseth and K. M. Marstokk, J. Mol. Struct. **13**, 191 (1972).

Chlorocyanoacetylene

C_3ClN $Cl—C^1≡C^2—C^3≡N$ $C_{\infty v}$

Bond	Substitution
CCl	1.625 B
C^1C^2	1.209 B
C^2C^3	1.369 B
CN	1.160 A

[1] T. Bjorvatten, J. Mol. Struct. **20**, 75 (1974).

3,3,3-Trifluoro-1-Propyne

C_3HF_3 $H—C≡C—CF_3$ C_{3v}

Bond	Substitution	Effective	Angle	Effective
HC	1.056 B		FCF	107.5 X
C≡C	1.201 A			
C—C		1.464 X		
CF		1.335 X		

[1] N. N. Shoolery, R. G. Shulman, W. F. Sheehan, Jr., V. Schomaker, and D. M. Yost, J. Chem. Phys. **19**, 1364 (1951).

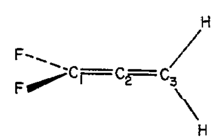
2-Propynenitrile

C_3HN HCCCN $C_{\infty v}$

Bond	Substitution	Effective
CH	1.058 A	1.057 A
C≡C	1.205 A	1.203 A
C—C	1.378 A	1.382 A
CN	1.159 A	1.157 A

[1] A. A. Westenberg and E. B. Wilson, Jr., J. Am. Chem. Soc. **72**, 199 (1950).
[2] J. K. Tyler and J. Sheridan, Trans. Faraday Soc. **59**, 2661 (1963).

1,1-Difluoroallene

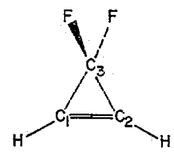


$C_3H_2F_2$ C_{2v}

Bond	Effective	Substitution	Angle	Effective	Substitution
C_2C_3		1.306 B	HCH		117.8 B
CH		1.086 B	CCH		121.1 B
C_1C_2	1.302 D		FCF	110.2 D	
CF	1.323 D		CCF	124.9 D	

[1] J. R. Durig, Y. S. Li, C. C. Tong, A. P. Zens and P. D. Ellis, J. Am. Chem. Soc. **96**, 3805 (1974).

3,3-difluorocyclopropene



$C_3H_2F_2$ C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
C_1C_2	1.321 A		FCF		105.5 D
CH	1.075 A		$C_1C_3C_2$		54.6 C
C_1C_3		1.438 C	HC_1C_2	148.4 A	
CF		1.365 C			

[1] K. R. Ramaprasad, V. W. Laurie, and N. C. Craig, J. Chem. Phys. **64**, 4832 (1976).

Malononitrile

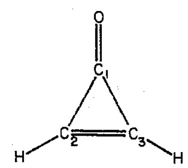
$C_3H_2N_2$ $CH_2(CN)_2$ C_{2v}

Bond	Effective	Angle	Effective
CC	1.47 E	CCC	109 E
CN	1.17 E	HCH	109 E
CH	1.09 D	CCN[a]	174 E

[a] The cyano group is bent outward.

[1] E. Hirota and Y. Morino, Bull. Chem. Soc. Japan **33**, 705 (1960).
[2] E. Hirota and Y. Morino, Bull. Chem. Soc. Japan **33**, 158 (1960).

Cyclopropenone

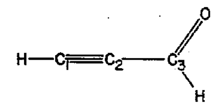


C_3H_2O C_{2v}

Bond	Substitution	Angle	Substitution
CO	1.212 B	HC_2C_3	144.9 B
C_1C_2	1.412 C	$C_2C_3C_1$	62.6 B
C_2C_3	1.302 B		
CH	1.097 C		

[1] R. C. Benson, W. H. Flygare, M. Oda and R. Breslow, J. Am. Chem Soc. **95**, 2772 (1973).

2-Propynal



C_3H_2O C_s

Bond	Substitution	Average	Angle	Substitution	Average
HC_1	1.055 B	1.054 C	C_2C_3O	123.9 D	124.2 B
HC_3	1.106 B	1.114 C	C_2C_3H	113.9 D	113.8 D
C_1C_2	1.209 B	1.205 C	$C_1C_2C_3$	178.4 E[a]	178.6 C
C_2C_3	1.444 B	1.449 A	HC_1C_2	180.0 E	
C_3O	1.214 B	1.212 B			

[a] The tilt is toward the aldehydic hydrogen.

[1] C. C. Costain and J. R. Morton, J. Chem. Phys. **31**, 389 (1959).
[2] M. Sugie, T. Kukuyama and K. Kuchitsu, J. Mol. Struct. **14**, 333 (1972).

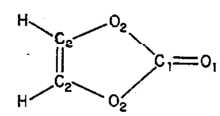
Propiolic Acid
(Propargylic or Propynoic Acid)

$C_3H_2O_2$ HC≡CCOOH C_s

It was determined that the species is planar with the hydroxyl hydrogen *cis* to the carbonyl group.

[1] D. G. Lister and J. K. Tyler, Spectrochim. Acta **28A**, 1423 (1972).

Cyclic Vinylene Ester (Vinylene Carbonate)



$C_3H_2O_3$ C_{2v}

Bond	Substitution	Angle	Substitution
C_2C_2	1.331 A	$C_2C_2O_2$	108.6 X
C_2O_2	1.385 X	$C_2O_2C_1$	106.9 X
C_1O_2	1.364 X	$O_2C_1O_2$	108.8 X
C_1O_1	1.191 A		

[1] W. F. White and J. E. Boggs, J. Chem. Phys. **54**, 4714 (1971).

3-Bromopropyne (Propargyl bromide)

C_3H_3Br $BrH_2C^3C^2{\equiv}C^1H$ C_s

Bond	Effective	Angle	Effective
C^3Br	1.94 E	C^2C^3Br	112 E
C^2C^3	1.46 E		

Four isotopic species studied; C^1H, C^3H, $C^2{\equiv}C^1$ and C^2C^3H values were assumed.

[1] Y. Kikuchi, E. Hirota and Y. Morino, Bull. Chem. Soc. Japan 34, 348 (1961).

3-Chloropropyne (Propargyl Chloride)

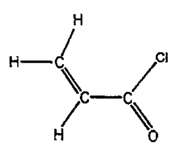
C_3H_3Cl $ClH_2C^3C^2{\equiv}C^1H$ C_s

Bond	Effective	Angle	Effective
CCl	1.780 E	CCCl	111.9 E
C^2C^3	1.465 E	HCH	108.7 D
		C^2C^3H	111.5 E

Four isotopic species studied; C^1H, C^3H, $C^2{\equiv}C^1$ bond lengths were assumed.

[1] E. Hirota and Y. Morino, Bull. Chem. Soc. Japan 34, 341 (1961).

trans-Propenoyl Chloride (*trans*-Acryloyl Chloride)

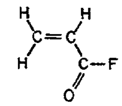


C_3H_3ClO C_s

Spectra were assigned for one isomer, established as the s-trans conformer as shown in the figure. Evidence for a second conformer (cis or possibly gauche) was discussed but no assignment was obtained.

[1] R. Kewley, D. C. Hemphill, and R. F. Curl, Jr., J. Mol. Spectrosc. 44, 443 (1972).

cis-Propenoyl Fluoride (*cis*-Acryloyl Fluoride)



C_3H_3FO C_s

Existence of two planar rotational isomers was established. One isotopic species was assigned for each isomer and rotational constants were determined. Although the authors proposed structures consistent with rotational constants, they could not positively determine which isomer was *cis* and which was *trans*. Figure shows *cis* form; see acryloyl chloride for *trans* form.

[1] J. J. Keirns and R. F. Curl, Jr., J. Chem. Phys. 48, 3773 (1968).

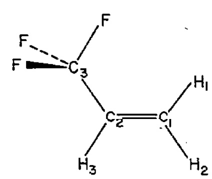
cis-1,2,3-Trifluorocyclopropane

$C_3H_3F_3$ HFC—HFC—HFC C_{3v}

Bond	Substitution	Effective	Angle	Effective
CC	1.567 B		HCF	112.3 B
CH	1.095 B			
CF		1.354 B		

[1] C. W. Gillies, J. Mol. Spectrosc. 59, 482 (1976).

3,3,3-Trifluoro-1-propene



$C_3H_3F_3$ C_s

Bond	Effective	Angle	Effective
C_2C_3	1.489 B	FCF	106.8 C
C_1C_2	1.312 C	$C_3C_2C_1$	124.8 C
CH_1	1.085 C	CCH_1	120.6 D
CH_2	1.092 C	CCH_2	122.8 D
CH_3	1.109 B	$C_1C_2H_3$	121.2 D
CF[a]	1.345 B	θ[b]	1.0 D

[a] Assumed value.

[b] Tilt angle of the CF_3 symmetry axis from C—C bond axis and away from the double bond.

[1] S. Saito and F. Makino, Bull. Chem. Soc., Japan 47, 1863 (1974).

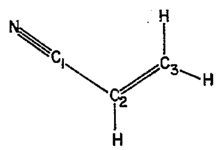
Trifluoroacetic Acid-Formic Acid Dimer

$C_3H_3F_3O_4$ $CF_3CO_2H \cdot HCO_2H$ C_s

Bond	Effective
O···O	2.67 X

[1] C. C. Costain and G. P. Srivastava, J. Chem. Phys. 41, 1620 (1964).

Vinyl cyanide



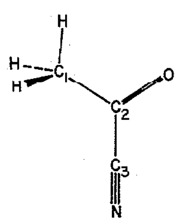
C_3H_3N C_s

Bond	Substitution	Angle	Substitution
CN	1.164 B	$C_1C_2C_3$	122.6 C
C_1C_2	1.426 B	HC_2C_3	121.7 B
C_2C_3	1.339 B		
C_2H	1.086 B		

C_2C_1N was linear to within experimental accuracy.

[1] C. C. Costain and B. P. Stoicheff, J. Chem. Phys. 30, 777 (1959).

Acetyl cyanide



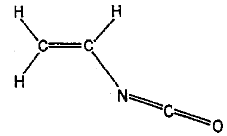
C_3H_3NO C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
CO	1.226 D		C_1C_2O	124.0 D	
C_1C_2	1.490 D		$C_1C_2C_3$	115.0 D	
C_2C_3	1.466 C		HCH		108.7 C
CN	1.164 C				
CH		1.086 C			

C_2C_3N group was assumed to be linear, and the methyl group was assumed to be symmetrical.

[1] L. C. Krisher and E. B. Wilson, J. Chem. Phys., 31, 882 (1959).

Isocyanoethene (Vinyl isocyanate)

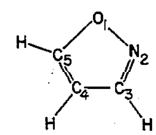


C_3H_3NO C_s

Microwave data confirm the planar *trans* conformation of the molecule.

[1] A. Bouchy and G. Roussy, C. R. Acad. Sci. Paris 284, 411 (1977).

Isoxazole

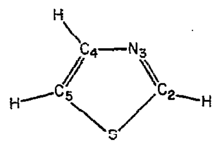


C_3H_3NO C_s

Bond	Substitution	Angle	Substitution
O_1N_2	1.399 A	$C_5O_1N_2$	108.9 A
N_2C_3	1.308 A	$O_1N_2C_3$	105.3 A
C_3C_4	1.426 A	$N_2C_3C_4$	112.3 A
C_4C_5	1.357 A	$C_3C_4C_5$	103.0 A
C_5O_1	1.344 A	$C_4C_5O_1$	110.5 A
C_3H	1.078 B	C_4C_3H	129.1 B
C_4H	1.074 B	C_3C_4H	128.5 B
C_5H	1.074 B	C_4C_5H	133.4 B

[1] O. L. Stiefvater, J. Chem. Phys. 63, 2560 (1975).
[2] O. L. Stiefvater, P. Nosberger and J. Sheridan, Chem. Phys. 9, 435 (1974).

Thiazole



C_3H_3NS C_s

Bond	Substitution	Angle	Substitution
SC_2	1.724 X	C_5SC_2	89.3 X
C_2N	1.304 X	SC_2N	115.1 X
NC_4	1.372 A	C_2NC_4	110.1 X
C_4C_5	1.367 X	NC_4C_5	115.8 X
C_5S	1.713 X	C_4C_5S	109.5 X
C_2H_2	1.077 X	SC_2H_2	121.2 X
C_4H_4	1.080 A	NC_2H_2	123.5 X
C_5H_5	1.076 X	NC_4H_4	119.3 A
		$C_5C_4H_4$	124.8 X
		$C_4C_5H_5$	129.0 X
		SC_5H_5	121.4 X

Uncertain structural data caused by a number of small substitution coordinates.

[1] L. Nygaard, E. Asmussen, J. H. Høg, R. C. Maheshwari, C. H. Nielsen, I. B. Petersen, J. Rastrup-Andersen, and G. O. Sørensen, J. Mol. Struct. **8**, 225 (1971).

s-Triazine

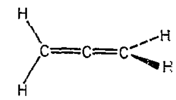
$C_3H_3N_3$ N=CH—N=CH—N=CH D_{3h}

Bond	Effective	Angle	Effective
CN	1.338 X	NCN	127 X
		CNC	113 X

In order to obtain the structural parameters it was necessary to assume the CH bond distances. Since the uncertainties in the other parameters are dependent upon this assumption, their uncertainties are given an X rating.

[1] J. E. Lancaster and B. P. Stoicheff, Can. J. Phys. **34**, 1016 (1956).

Allene

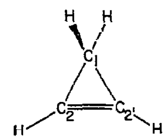


C_3H_4 D_{2d}

Bond	Effective	Angle	Effective
CH	1.085 B	HCH	118.5 B
CC	1.309 A		

[1] A. G. Maki and R. A. Toth, J. Mol. Spectrosc. **17**, 136 (1965).
[2] R. J. Butcher and W. J. Jones, J. Raman Spectrosc. **1**, 393 (1973).

Cyclopropene



C_3H_4 C_{2v}

Bond	Substitution	Angle	Substitution
C_1C_2	1.509 B	$C_1C_2C_{2'}$	50.8 A
$C_2C_{2'}$	1.296 A	$C_2C_{2'}H$	149.9 B
C_2H	1.072 B	HCH	114.6 B
C_1H	1.088 B		

[1] W. M. Stigliani, V. W. Laurie and J. C. Li, J. Chem. Phys. **62**, 1890 (1975).
[2] P. H. Kasai, R. J. Myers, D. F. Eggers and K. B. Wiberg, J. Chem. Phys. **30**, 512 (1959).

Methyl acetylene

C_3H_4 $H_3C^1—C^2≡C^3—H$ C_{3v}

Bond	Substitution	Angle	Substitution
C^1C^2	1.459 B	HC^1C^2	110.2 B
C^2C^3	1.206 B		
C^3H	1.056 B		
C^1H	1.105 B		

[1] C. C. Costain, J. Chem. Phys. **29**, 864 (1958).
[2] R. Trambarulo and W. Gordy, J. Chem. Phys. **18**, 1613 (1950).
[3] L. F. Thomas, E. I. Sherrard and J. Sheridan, Trans. Faraday Soc. **51**, 619 (1955).

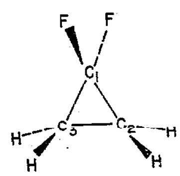
1,1-Dichlorocyclopropane

$C_3H_4Cl_2$ $Cl_2C^1—C^2H_2—C^3H_2$ C_{2v}

Bond	Substitution	Angle	Substitution
CH	1.085 B	HCH	117.5 B
C^2C^3	1.534 B	C^2C^3H	117.5 B
C^1C^2	1.532 C	ClCCl	114.2 C
CCl	1.734 C	$C^2C^1C^3$	60.1 B

[1] W. H. Flygare, A. Narath, and W. D. Gwinn, J. Chem. Phys. **36**, 200 (1962).

1,1-Difluorocyclopropane



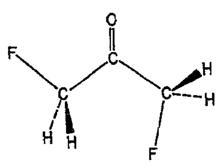
$C_3H_4F_2$ C_{2v}

Bond	Substitution	Angle	Substitution
C_1C_2	1.464 C	FCF	108.3 C
C_2C_3	1.553 A	HCH	116.9 B
CF	1.355 C		
CH	1.082 B		

Structural parameters were evaluated for the D_4 species.

[1] A. T. Perretta and V. W. Laurie, J. Chem. Phys. **62**, 2469 (1975).

1,3-Difluoroacetone

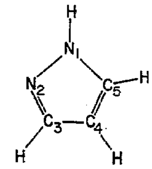


$C_3H_4F_2O$ C_s

The observed spectra were consistent with the above conformation. Intensity measurements suggest that this species may represent only about 20% of the gas-phase sample.

[1] D. J. Finnigan, C. W. Gillies, R. D. Suenram and E. B. Wilson, J. Mol. Spectrosc. **57**, 363 (1975).

Pyrazole

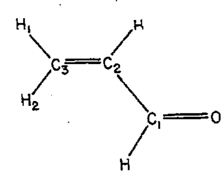


$C_3H_4N_2$ C_s

Bond	Substitution	Angle	Substitution
N_1N_2	1.349 B	$N_1N_2C_3$	104.1 B
N_2C_3	1.331 B	$N_2C_3C_4$	111.9 B
C_3C_4	1.416 B	$C_3C_4C_5$	104.5 B
C_4C_5	1.372 A	$C_4C_5N_1$	106.4 B
C_5N_1	1.359 B	$C_5N_1N_2$	113.1 B
N_1H	0.998 B	N_2C_3H	119.3 B
C_3H	1.078 B	C_3C_4H	127.9 B
C_4H	1.076 B	N_1C_5H	121.5 B
C_5H	1.077 B	N_2N_1H	118.4 B

[1] L. Nygaard, D. Christen, J. T. Nielsen, E. J. Pedersen, O. Snerling, E. Vestergaard and G. O. Sorensen, J. Mol. Struct. **22**, 401 (1974).

trans-Acrolein



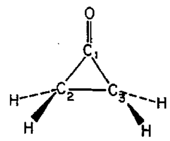
C_3H_4O C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
CO	1.219 C		CCO	123.3 C	
C_1C_2	1.470 B		C_2C_1H	115.1 B	
C_1H	1.108 B		C_1C_2H	117.3 B	
C_2H	1.084 B		$C_1C_2C_3$		119.8 C
C_2C_3		1.345 B	$C_2C_3H_1$		121.5 C
C_3H_1		1.086 C	$C_2C_3H_2$		120.0 C
C_3H_2		1.086 C			

The C_3H_1 and C_3H_2 distances have been assumed to be equal.

[1] E. A. Cherniak and C. C. Costain, J. Chem. Phys. **45**, 104 (1966).

Cyclopropanone

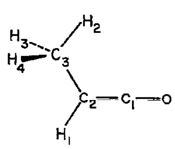


C_3H_4O C_{2v}

Bond	Substitution	Angle	Substitution
CO	1.191 E	$C_1C_2C_3$	57.7 C
C_1C_2	1.475 D	$C_2C_1C_3$	64.6 C
C_2C_3	1.575 D	HCH	114.1 D
CH	1.086 D	HC_2C_1	118.5 D
		HC_2C_3	118.3 D

[1] J. M. Pochan, J. E. Baldwin and W. H. Flygare, J. Amer. Chem. Soc. **91**, 1896 (1969).
[2] J. M. Pochan, J. E. Baldwin and W. H. Flygare, J. Amer. Chem. Soc. **90**, 1072 (1968).

Methyl ketene



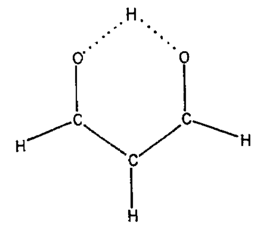
C_3H_4O C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
C_1O	1.171 B		OC_1C_2	179.5 C	
C_1C_2	1.306 B		$C_1C_2C_3$	122.6 B	
C_2C_3	1.518 B		$C_1C_2H_1$	123.7 B	
C_2H_1	1.083 B		$C_2C_3H_2$	111.1 B	
C_3H_2	1.083 B		$C_2C_3H_3$		110.7[a] C
C_3H_3		1.094[a] C	$H_3C_3H_4$		107.9[a] C

[a] Recalculated from the original data.

[1] B. Bak, J. J. Christiansen, K. Kunstmann, L. Nygaard and J. Rastrup-Andersen, J. Chem. Phys. **45**, 883 (1966).

Malonaldehyde

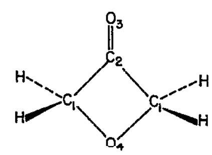


$C_3H_4O_2$ C_{2v}

Experimental evidence supports a structure with average C_{2v} symmetry. A low-barrier double-minimum hydrogen-bond potential function may exist. The O···O distance was found to be 2.55 (X).

[1] W. F. Rowe, Jr., R. W. Duerst, and E. B. Wilson, J. Amer. Chem. Soc. **98**, 4021 (1976).

3-Oxetanone



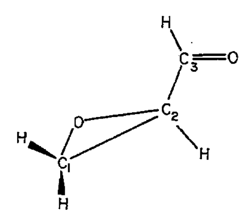
$C_3H_4O_2$ C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
C_1C_2	1.522 B		$C_1C_2C_1$	88.1 B	
C_1O_4[a]		1.450 X	$C_2C_1O_4$[a]		88.5 X
C_2O_3[a]		1.230 X	$C_1O_4C_1$[a]		94.8 X

[a] In order to obtain parameters involving oxygen atoms, the methylene group parameters were assumed.

[1] J. S. Gibson and D. O. Harris, J. Chem. Phys. **57**, 2318 (1972).

Oxiranecarboxaldehyde

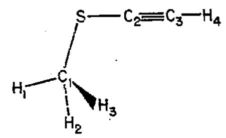


$C_3H_4O_2$ C_1

Bond	Substitution	Angle	Substitution
C_1C_2	1.453 E	$C_1C_2C_3$	119.8 D
C_2C_3	1.469 C		

[1] R. A. Creswell, P. J. Manor, R. A. Assink and R. H. Schwendeman, J. Mol. Spectrosc. **64**, 365 (1977).

Ethynyl Methyl Sulfide



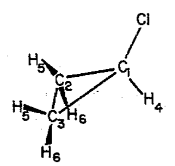
C_3H_4S C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
SC_1	1.813 B		C_1SC_2		99.9 C
SC_2		1.685 C	$H_1C_1H_2$	110.0 B	
C_2C_3		1.205 C	SC_2C_3		178.0 C
C_3H_4		1.061 C	$H_2C_1H_3$	110.3 B	
C_1H_1	1.079 B				
C_1H_2	1.090 B				

The $C_2C_3H_4$ angle was assumed to be 180°. The acetylene group is tilted away from the methyl group. The methyl group is tilted approximately 2° away from the acetylene group.

[1] D. den Engelsen, J. Mol. Spectrosc. **30**, 474 (1969).
[2] D. den Engelsen, J. Mol. Spectrosc. **22**, 426 (1967).

Chlorocyclopropane (Cyclopropyl chloride)



C_3H_5Cl C_s

Bond	Substitution	Angle	Substitution
CCl	1.740 C	CCCl	118.7 C
C_1C_2	1.513 C	ClCH	115.8 C
C_2C_3	1.515 B	CCH_4	116.1 C
CH_4	1.079 B	$C_1C_3H_5$	115.5 C
CH_5	1.086 C	$C_1C_3H_6$	117.8 C
CH_6	1.082 C	$C_2C_3H_5$	116.9 C
		$C_2C_3H_6$	118.7 C
		HCH	116.2 C

[1] R. H. Schwendeman, G. D. Jacobs and T. M. Krigas, J. Chem. Phys. **40**, 1022 (1964).

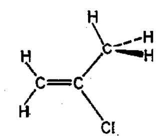
cis-1-Chloropropene

C_3H_5Cl $CH_3—CH=CHCl$ C_s

Assuming all other parameters to be the same as in propene, C—Cl = 1.735 (X) and C=C—Cl = 125.2 (X). A *trans* form was also investigated and similar assumptions led to C—Cl = 1.728 (X) and C=C—Cl = 121.9 (X).

[1] R. A. Beaudet, J. Chem. Phys. **40**, 2705 (1964).
[2] R. A. Beaudet, J. Chem. Phys. **37**, 2398 (1962).

2-Chloropropene

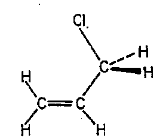


C_3H_5Cl C_s

The equilibrium conformation of the methyl group was found to be that given in figure. The authors have also given a reasonable structure based on assumed parameters from propene and vinyl chloride.

[1] W. Good, R. J. Conan, A. Bauder and Hs. H. Gunthard, J. Mol. Spectrosc. **41**, 381 (1972).
[2] M. L. Unland, V. Weiss and W. H. Flygare, J. Chem. Phys. **42**, 2138 (1965).

cis-3-Chloropropene



C_3H_5Cl C_s

Rotational constants for two chlorine isotopic species were in agreement with a plane of symmetry. A second rotamer, with a dihedral angle of 122° about C—C bond, was also observed.

[1] E. Hirota, J. Mol. Spectrosc. **35**, 9 (1970).

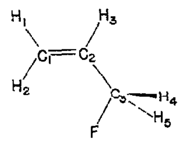
Propanoyl Chloride (Propionyl Chloride)

C_3H_5ClO CH_3CH_2COCl C_s

The most stable isomer was determined as a heavy atom planar configuration with the methyl group and the carbonyl oxygen atom *cis* to each other.

[1] H. Karlsson, J. Mol. Struct. **33**, 227 (1976).

cis-3-Fluoropropene



C_3H_5F C_s

Bond	Substitution	Angle	Substitution
C_1C_2	1.333 C	$C_1C_2C_3$	124.6 C
C_2C_3	1.488 C	C_2C_3F	111.7 C
C_3F	1.382 C	$C_2C_1H_1$	120.9 C
C_1H_1	1.080 C	$C_2C_1H_2$	119.2 C
C_1H_2	1.105 C	$H_1C_1H_2$	119.9 C
C_3H_4	1.098 C	$C_2C_3H_4$	111.1 C
C_3H_5	1.098 C	$C_2C_3H_5$	111.1 C
		$H_4C_3H_5$	108.1 C
		H_4C_3F	107.4 C
		H_5C_3F	107.4 C

C_2H_3 and $C_1C_2H_3$ parameters assumed.

[1] E. Hirota, J. Chem. Phys. **42**, 2071 (1965).

gauche-3-Fluoropropene

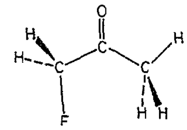
C_3H_5F $CH_2{=}CHCH_2F$ C_1

Bond	Substitution	Angle	Substitution
C_1C_2	1.354 D	$C_1C_2C_3$	121.6 D
C_2C_3	1.486 D	C_2C_3F	110.9 D
C_3F	1.371 D	$C_2C_1H_1$	119.2 D
C_1H_1	1.098 D	$C_2C_1H_2$	121.5 D
C_1H_2	1.054 D	$H_1C_1H_2$	119.3 D
C_3H_4	1.127 D	$C_2C_3H_4$	107.4 D
C_3H_5	1.137 D	$C_2C_3H_5$	105.2 D
		$H_4C_3H_5$	111.4 D
		H_4C_3F	107.1 D
		H_5C_3F	114.7 D
		Dihedral[a]	127.1

Gauche form has CH_2F rotated 127.1 relative to *cis*. See *cis*-3-fluoropropene structure. C_2H_3 and $C_1C_2H_3$ parameters assumed.

[1] E. Hirota, J. Chem. Phys. **42**, 2071 (1965).

1-Fluoro-2-propanone (Fluoroacetone)

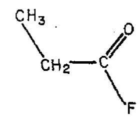


C_3H_5FO C_s

No quantitative structural information other than the conformation of the most stable rotamer was obtained.

[1] E. Saegerbarth and L. Krisher, J. Chem. Phys. **52**, 3555 (1970).

cis-Propionyl Fluoride



C_3H_5FO C_s

Other than establishing this conformation as the most stable, no quantitative information was obtained about the structure.

A *gauche* form, 1290 cal/mol less stable, was also observed. See the following.

[1] O. Stiefvater and E. B. Wilson, J. Chem. Phys. **50**, 5385 (1969).

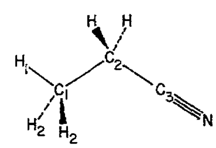
gauche-Propionyl Fluoride

C_3H_5FO CH_3CH_2COF C_1

Dihedral angle between CCC and COF plane is 120° (E). A *cis* form, 1290 cal/mol more stable, was also observed. See the preceding.

[1] O. Stiefvater and E. B. Wilson, J. Chem. Phys. **50**, 5385 (1969).

Propanenitrile (Ethyl cyanide)



C_3H_5N C_s

Bond	Substitution	Angle	Substitution
C_1C_2	1.537 B	C_2C_3N	178.7[a] D
C_2C_3	1.459 C	$C_1C_2C_3$	112.0 B
CN	1.159 C	C_1C_2H	110.6 B
C_2H	1.094 B	HC_2C_3	108.1 B
C_1H_1	1.079 D	HC_2H	107.2 B
C_1H_2	1.091 B	$H_2C_1H_2$	107.8 B
		$H_2C_1C_2$	110.5 B
		$H_1C_1C_2$	110.1 E

[a] The CN group is bent slightly toward the methyl group.

[1] H. M. Heise, H. Lutz and H. Dreizler, Z. Naturforsch. **29a**, 1345 (1974).

Nitrocyclopropane

$C_3H_5NO_2$	$\overline{CH_2CH_2CHNO_2}$	C_s

The conformation of the molecule is found to be the bisected one with the plane of the nitro group perpendicular to the plane of the cyclopropyl ring.

[1] A. R. Mochel, C. O. Britt, and J. E. Boggs, J. Chem. Phys. 58, 3221 (1973).

Ethyl Thiocyanate

C_3H_5NS	CH_3CH_2SCN	C_1

One rotational isomer, having the CH_3 group and SCN group *gauche* to one another, was identified.

[1] A. Bjørseth and K. M. Marstokk, J. Mol. Struct. 11, 15 (1972).

Cyclopropane

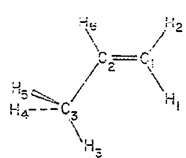
C_3H_6	$\underline{CH_2CH_2CH_2}$	D_{3h}

Bond	Effective	Angle	Effective
CH	1.083 C	HCH	114.0 C
CC	1.512 C		

In the calculation, $r_0(C—H) - r_0(C—D) = 0.002$ Å was assumed.

[1] R. J. Butcher and W. J. Jones, J. Mol. Spectrosc. 47, 64 (1973).
[2] W. J. Jones and B. P. Stoicheff, Can. J. Phys. 42, 2259 (1964).

Propene (Propylene)



C_3H_6	C_s

Bond	Substitution	Angle	Substitution
C_1C_2	1.336 B	$H_4C_3H_5$	106.2 D
C_2C_3	1.501 B	$H_1C_1H_2$	118.0 B
C_1H_1	1.091 B	$H_1C_1C_2$	120.5 B
C_1H_2	1.081 B	$H_2C_1C_2$	121.5 B
C_2H_6	1.090 B	$C_1C_2C_3$	124.3 B
C_3H_3	1.085 B	$H_6C_2C_3$	116.7 B
$C_3H_{4,5}$	1.098 D	$H_6C_2C_1$	119.0 B
		$H_3C_3H_4$	109.0 D
		$H_3C_3C_2$	111.2 B

[1] D. R. Lide and D. Christensen, J. Chem. Phys. 35, 1374 (1961).
[2] E. Hirota and Y. Morino, J. Chem. Phys. 45, 2326 (1966).

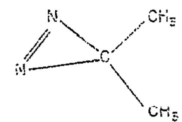
Dimethylcyanamide

$C_3H_6N_2$	$(CH_3)_2NCN$	C_s

It was shown that the heavy atom skeleton is non-planar.

[1] Y. S. Li and J. R. Durig, J. Mol. Struct. 16, 433 (1973).

3,3-Dimethyl Diazirine



$C_3H_6N_2$	C_{2v}

Bond	Effective	Angle	Effective
CC	1.50 X	CCC	120 X
CN	1.49 X	H_sCH_s	109 X
NN	1.235 B	H_aCH_a	108 X
CH_s	1.08 X		
CH_a	1.10 X		

NCN and NNC angles assumed. H_s and H_a refer to hydrogen atoms in and out of the plane of symmetry, respectively.

[1] J. E. Wollrab, L. H. Sharpen, D. P. Ames, and J. A. Merritt, J. Chem. Phys. 49, 2405 (1968).

Acetone

C_3H_6O	CH_3COCH_3	C_{2v}

Bond	Substitution	Angle	Substitution
CC	1.507 B	CCC	117.2 B
CO	1.222 B	HCH	108.7 B
CH	1.085 C	2θ	119.9 B

Methyl group assumed to be symmetrical. Internal rotation analysis provided 2θ, the angle between symmetry axes of methyl groups.

[1] R. Nelson and L. Pierce, J. Mol. Spectrosc. 18, 344 (1965).
[2] J. D. Swalen and C. C. Costain, J. Chem. Phys. 31, 1562 (1959).

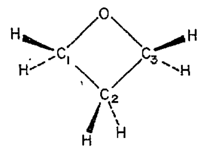
Allyl Alcohol

C_3H_6O	$CH_2{=}CHCH_2OH$	C_1

Molecule has gauche conformation. OH lies out of the plane and points toward the double bond.

[1] A. N. Murty and R. F. Curl, Jr., J. Chem. Phys. 46, 4176 (1967).

Oxetane (Trimethylene Oxide)



C_3H_6O C_s

Bond	Effective	Angle	Effective
C_1C_2	1.549 C	HC_2H	110.7 C
C_1O	1.449 C	HC_1H	110.3 C
C_1H	1.091 C	$C_1C_2C_3$	84.6 C
C_2H	1.100 C	C_1OC_3	92.0 C
		C_2C_1O	91.7 C

Because of low barrier, the effective symmetry is C_{2v}.

[1] S. I. Chan. J. Zinn and W. D. Gwinn, J. Chem. Phys. **34**, 1319 (1961).

cis-Propionaldehyde

C_3H_6O CH_3CH_2CHO C_s

Gauche form also observed. Carbonyl eclipses methyl group but no detailed structure available.

[1] S. S. Butcher and E. B. Wilson, J. Chem. Phys. **40**, 1671 (1964).

gauche-Propionaldehyde

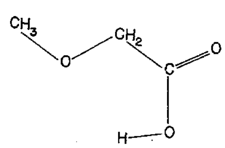
C_3H_6O CH_3CH_2CHO C_1

Angle	Effective
θ^a	131 X

[a] θ is angle of rotation of carbonyl group from *cis* conformation where carbonyl eclipses methyl group.

[1] S. S. Butcher and E. B. Wilson, J. Chem. Phys. **40**, 1671 (1964).

Methoxyacetic Acid

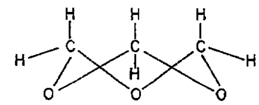


$C_3H_6O_3$ C_s

Symmetry plane and conformation seem well established, but no detailed structure is available.

[1] K. M. Marstokk and H. Mollendal, J. Mol. Struct. **18**, 247 (1973).

s-Trioxane



$C_3H_6O_3$ C_{3v}

Bond	Substitution	Angle	Substitution
CO	1.420 C	OCO	112.0 C
		COC	109.5 C

[1] J. M. Colmont, J. Mol. Struct. **21**, 387 (1974).
[2] T. Oka, K. Tsuchiya, S. Iwata and Y. Morino, Bull. Chem. Soc. Japan **37**, 4 (1964).

Methyl Vinyl Sulfide

C_3H_6S $CH_3SCH{=}CH_2$ C_s

Cis conformation (with planar heavy atoms) was definitely established.

[1] R. E. Penn and R. F. Curl, Jr., J. Mol. Spectrosc. **24**, 235 (1967).

2-Propene-1-thiol (Allyl Mercaptan)

C_3H_6S $CH_2{=}CHCH_2SH$ C_1

Angle	Effective
α	124 X
β	50 X

Only gauche form exists. With α and β defined as zero in hypothetical *cis* form, the observed gauche form is estimated to have the above values of α and β, the sense being such that vinyl and thiol groups, respectively, are rotated above the plane of the paper.

[1] K. V. L. N. Sastry, S. C. Dass, W. V. F. Brooks, and A. Bhaumitt, J. Mol. Spectrosc. **31**, 54 (1969).

Selenetane (Trimethylene Selenide)

C_3H_6Se $CH_2{-}CH_2{-}CH_2{-}Se$ (ring) C_s

Angle	Effective
Dihedral	29.5 X

Various assumptions about vibrational motion required to obtain dihedral angle estimate.

[1] M. G. Petit, J. S. Gibson, and D. O. Harris, J. Chem. Phys. **53**, 3408 (1970).

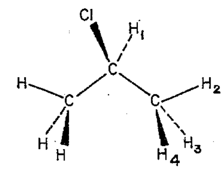
2-Bromopropane

C_3H_7Br $CH_3CHBrCH_3$ C_s

Bond	Substitution	Angle	Substitution
CBr	1.957 B	CCBr	110.0 B
CC	1.508 D	CCC	114.2 C

[1] R. H. Schwendeman and F. L. Tobiason, J. Chem. Phys. 43, 201 (1965).

2-Chloropropane

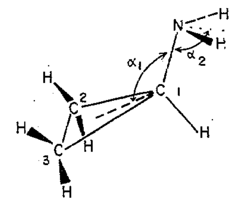


C_3H_7Cl C_s

Bond	Substitution	Angle	Substitution
CCl	1.798 C	CCC	112.5 C
CC	1.523 C	CCCl	109.3 B
CH_1	1.091 B	CCH_1	110.1 B
$CH_{2,3,4}$	1.092 C	$ClCH_1$	105.4 C
		CCH_2	110.7 C
		$CCH_{3,4}$	109.7 C
		H_3CH_4	109.1 C
		H_2CH_3	109.1 C
		H_2CH_4	108.7 C

[1] F. L. Tobiason and R. H. Schwendeman, J. Chem. Phys. 40, 1014 (1964).

Cyclopropaneamine (Cyclopropylamine)



C_3H_7N C_s

Bond	Substitution	Effective[a]	Angle	Substitution	Effective[a]
C_1C_2	1.486 C		$C_2C_1C_3$	61.2 B	
C_2C_3	1.513 B		CCN		116.3 C
CN		1.462 D	CNH		111.0 E
NH		1.008 D	HNH		108.1 D
H···H	1.632 B		α_1		121.0 C
			α_2		127.5 X

[a] All CH parameters were assumed to obtain these values. Uncertainties reflect a reasonable range for the assumed parameters.

[1] D. K. Hendricksen and M. D. Harmony, J. Chem. Phys. 51, 700 (1969).
[2] M. D. Harmony, R. E. Bostrom and D. K. Hendricksen, J. Chem. Phys. 62, 1599 (1975).
[3] M. D. Harmony, personal communication.

2-Methylaziridine (*trans*-Propyleneimine)

C_3H_7N HN—CH_2—CH—CH_3 (ring) C_1

Methyl group *trans* to hydrogen on nitrogen.

[1] Y. S. Li, M. D. Harmony, D. Hayes, and E. L. Beeson, Jr., J. Chem. Phys. 47, 4514 (1967).

Cyclopropylphosphine

C_3H_7P CH_2—CH_2—$CHPH_2$ (ring) C_s

C_s conformation confirmed; see cyclopropylamine.

[1] L. A. Dinsmore, C. O. Britt, and J. E. Boggs, J. Chem. Phys. 54, 915 (1971).

Propane

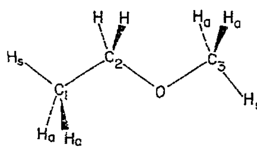
C_3H_8 — $CH_3CH_2CH_3$ — C_{2v}

Bond	Substitution	Angle	Substitution
CC	1.526 B	CCC	112.4 B
C_2H_2[a]	1.096 A	$H_2CH_{2'}$	106.1 A
C_1H_s[b]	1.089 C	H_aCH_a	107.3 C
C_1H_a	1.094 C	H_aCH_s	108.1 C
		CCH_s	111.8 C
		CCH_a	110.6 C

[a] C_2 is methylene carbon.
[b] H_s and H_a are in-plane and out-of-plane, respectively.

[1] D. R. Lide, Jr., J. Chem. Phys. 33, 1514 (1960).

trans-Ethylmethylether



C_3H_8O — C_s

Bond	Substitution	Angle	Substitution
C_1C_2	1.520 B	C_2OC_3	111.8 C
C_2O	1.404 C	C_1C_2O	108.2 C
C_3O	1.415 C	HC_2H	107.2 B
C_2H	1.101 B	C_1C_2H	110.9 B
C_3H_s	1.084 C	OC_3H_s	107.7 B
C_3H_a	1.100 B	OC_3H_a	111.0 C
C_1H_s	1.089 C	$H_aC_3H_a$	108.4 B
C_1H_a	1.092 B	$C_2C_1H_s$	110.5 B
		$C_2C_1H_a$	110.1 B
		$H_aC_1H_a$	108.6 B

[1] M. Hayashi and K. Kuwada, J. Mol. Struct. 28, 147 (1975).

n-Propyl Alcohol

C_3H_8O — $CH_3CH_2CH_2OH$

Both *trans* and *gauche* forms exist. Insufficient data for structural determination.

[1] L. M. Imanov, A. A. Abdurakhmanov and R. A. Ragimova, Opt. and Spectrosc. 25, 528 (1968).
[2] A. A. Abdurakhmanov, R. A. Ragimova and L. M. Imanov, Opt. and Spectrosc. 26, 75 (1969).

2-Methoxyethanol

$C_3H_8O_2$ — CH_3—O—CH_2—CH_2—OH — C_1

Conformation has been shown to be *gauche* about each of the CH_3O—C, C—C and C—OH bonds.

[1] P. Buckley and M. Brochu, Can. J. Chem. 50, 1149 (1972).

Trimethylarsine

C_3H_9As — $(CH_3)_3As$ — C_{3v}

Bond	Effective
CAs	1.959 D

Assumptions concerning angle CAsC and methyl group parameters have a relatively small effect upon the CAs distance.

[1] D. R. Lide, Spectrochim. Acta, 1959, 473 (1959).

Trimethylamine-Boron Trifluoride

$C_3H_9BF_3N$ — $(CH_3)_3NBF_3$ — C_{3v}

Bond	Substitution
BN	1.636 B

[1] P. S. Bryan and R. L. Kuczkowski, Inorg. Chem. 10, 200 (1971).

Bromotrimethylgermane

C_3H_9BrGe — $(CH_3)_3GeBr$ — C_{3v}

Bond	Substitution	Effective	Angle	Effective
GeBr	2.323 A		BrGeC[a]	106.3 C
GeC[a]		1.936 C		

[a] Methyl group parameters were assumed to obtain this parameter.

[1] Y. S. Li and J. R. Durig, Inorg. Chem. 12, 306 (1973).

Trimethylchlorogermane

C_3H_9ClGe — $(CH_3)_3GeCl$ — C_{3v}

Bond	Substitution	Effective	Angle	Effective
GeCl	2.170 A		CGeCl	105.9 B
GeC		1.940 B		

Methyl group parameters were assumed (CH = 1.095, HCH = 109.5) to obtain effective parameters.

[1] J. R. Durig and K. L. Hellams, J. Mol. Struct. 29, 349 (1975).

Chlorotrimethylsilane
(Trimethylchlorosilane)

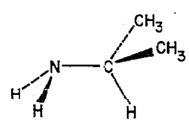
C_3H_9ClSi $(CH_3)_3SiCl$ C_{3v}

Bond	Effective	Angle	Effective
SiCl	2.022 E	ClSiC	110.5 D
SiC	1.857 D		

Methyl group parameters were assumed in order to obtain the other parameters.

[1] J. R. Durig, R. O. Carter, and Y. S. Li, J. Mol. Spectrosc. **44**, 18 (1972).

2-Aminopropane



C_3H_9N C_s

Isotopic substitution showed conclusively that amino group occupied the *trans* symmetrical position.

[1] S. C. Mehrota, L. L. Griffin, C. O. Britt and J. E. Boggs, J. Mol. Spectrosc. **64**, 244 (1977).

Trimethylamine

C_3H_9N $(CH_3)_3N$ C_{3v}

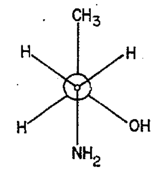
Bond	Substitution	Effective	Angle	Substitution	Effective
CN	1.451 B		CNC	110.9 C	
CH_1[a]	1.109 C		NCH_1	111.7 B	
CH_2		1.088 C	NCH_2		110.1 C
			H_1CH_2		108.1 C
			H_2CH_3		108.6 C

The H_2H_3 distance was assumed to be 1.7668 Å. The methyl groups are tilted 1.3° toward the nitrogen lone pair.

[a] H_1 lies in plane of symmetry; H_2 and H_3 are symmetrically situated out of plane.

[1] J. E. Wollrab and V. W. Laurie, J. Chem. Phys. **51**, 1580 (1969).
[2] D. R. Lide, Jr., and D. E. Mann, J. Chem. Phys. **28**, 572 (1958).

1-Amino-2-propanol



C_3H_9NO C_1

The microwave data were consistent with an intramolecularly hydrogen-bonded conformation as shown.

[1] K. M. Marstokk and H. Mollendal, J. Mol. Struct. **35**, 57 (1976).

Trimethylphosphine

C_3H_9P $(CH_3)_3P$ C_{3v}

Bond	Substitution	Effective	Angle	Effective
CH_s[a]	1.112 D		PCH_s	111.4 D
CH_a[a]		1.090 D	PCH_a	109.8 D
PC		1.843 C	H_sCH_a	108.2 D
			$H_aCH_{a'}$	109.4 D
			CPC	98.9 C

[a] s refers to in plane, a to out of plane.

[1] P. S. Bryan and R. L. Kuczkowski, J. Chem. Phys. **55**, 3049 (1971).

Trimethylgermane

$C_3H_{10}Ge$ $(CH_3)_3GeH$ C_{3v}

Bond	Substitution	Effective	Angle	Effective
GeH	1.522 C		CGeH[a]	109.3 C
GeC[a]		1.947 D		

[a] Methyl group parameters were assumed to obtain these parameters.

[1] J. R. Durig, M. M. Chen, Y. S. Li, and J. B. Turner, J. Phys. Chem. **77**, 227 (1973).

Trimethylsilane

$C_3H_{10}Si$ $(CH_3)_3SiH$ C_{3v}

Bond	Substitution	Effective	Angle	Substitution	Effective
SiC	1.868 B		CSiC	110.2 B	
SiH	1.489 B		HCH		107.9 C
CH		1.095 C			

The methyl groups are staggered with respect to the SiH bond, and have been assumed to be symmetric about the SiC bond.

[1] L. Pierce and D. H. Petersen, J. Chem. Phys. **33**, 907 (1960).

Trimethylamineborane

$C_3H_{12}BN$	$(CH_3)_3NBH_3$		C_{3v}
Bond	Substitution	Angle	Substitution
BN	1.638 C	CNB	109.9 C
CN	1.483 C	NBH	105.3 C
BH	1.211 C		

[1] P. Cassoux, R. L. Kuczkowski, P. S. Bryan, and R. C. Taylor, Inorg. Chem. **14**, 126 (1975).
[2] J. R. Durig, Y. S. Li, and J. Odom, J. Mol. Struct. **16**, 443 (1973).
[1] H. G. Schirdewahn, Doctoral Thesis, University of Freiburg, 1965.

Trimethylphosphineborane

$C_3H_{12}BP$		$(CH_3)_3PBH_3$			C_{3v}
Bond	Substitution	Effective	Angle	Substitution	Effective
PB[a]		1.901 D	CPC[a]		105.0 C
PC[a]		1.819 D	HCH[a]		109.3 D
CH[a]		1.08 D	HBH	113.5 C	
BH	1.212 D				

[a] In order to obtain these parameters, symmetrical CH_3 groups and the H---H distance in the methyl groups were assumed.

[1] P. S. Bryan and R. L. Kuczkowski, Inorg. Chem. **11**, 553 (1972).

Iodocyanoacetylene

C_3IN	$I—C^1\equiv C^2—C^3\equiv N$ $C_{\infty v}$
Bond	Substitution
CI	1.985 B
C^1C^2	1.207 B
C^2C^3	1.370 A
CN	1.160 A

[1] T. Bjorvatten, J. Mol. Struct. **20**, 75 (1974).

C_4 Molecules

Butadiyne (Diacetylene)

C_4H_2	$HC^1\equiv C^2—C^3\equiv C^4H$ $D_{\infty h}$
Bond	Effective
C^2C^3	1.376 X
C^1H	1.046 X

In order to calculate the structure it was necessary to assume the C≡C bond distance. The structural parameters listed above are rated X because of the uncertainty arising from this assumption.

[1] J. H. Callomon and B. P. Stoicheff, Can. J. Phys. **35**, 373 (1957).

1,1,1-Trifluoro-2-butyne

$C_4H_3F_3$		$F_3C^{(1)}—C^{(2)}\equiv C^{(3)}—C^{(4)}H_3$		C_{3v}
Bond	Substitution	Effective	Angle	Effective
CF		1.340 D	HCH	108.5 D
$C^{(1)}C^{(2)}$		1.455 D	FCF	106.1 D
$C^{(2)}C^{(3)}$		1.189 D		
$C^{(3)}C^{(4)}$	1.455 B			
CH		1.097[a]		

$C^{(1)}C^{(2)}$ distance assumed to be same as $C^{(3)}C^{(4)}$ distance.
[a] Assumed value.

[1] B. Bak, D. Christensen, L. Hansen-Nygaard and E. Tannenbaum, J. Chem. Phys. **26**, 241 (1957).

2-Butynenitrile (Methylcyanoacetylene)

C_4H_3N $CH_3—C\equiv C—CN$ C_{3v}

Molecular symmetry confirmed.

[1] J. Sheridan and L. F. Thomas, Nature **174**, 798 (1954).

Butatriene

C_4H_4	$C^1H_2=C^2=C^3=C^4H_2$ D_{2h}
Bond	Effective
C^2C^3	1.284 X

In order to derive the C^2C^3 bond distance it was necessary to assume HCH, C^3C^4, and C^1H. Because of the assumptions an estimate of the uncertainty in C^2C^3 can not be derived.

[1] B. P. Stoicheff, Can. J. Phys. **35**, 837 (1957).

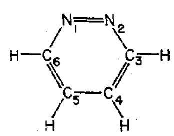
Trifluoroacetic Acid–Monofluoroacetic Acid Dimer

$C_4H_4F_4O_4$ $CF_3CO_2H \cdot CFH_2CO_2H$

Bond	Effective
O···O	2.69 X

[1] C. C. Costain and G. P. Srivastava, J. Chem. Phys. **41**, 1620 (1964).

Pyridazine

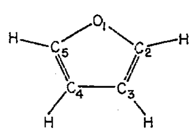


$C_4H_4N_2$ C_{2v}

Bond	Substitution	Angle	Substitution
NN	1.330 A	NNC	119.0 E
NC	1.353 E	NCC	123.7 E
C_3C_4	1.382 E	CCC	117.3 E
C_4C_5	1.375 A		

[1] W. Werner, H. Dreizler, and H. D. Rudolph, Z. Naturforsch. **22A**, 531 (1967).

Furan

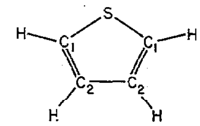


C_4H_4O C_{2v}

Bond	Substitution	Angle	Substitution
CO	1.362 B	C_5OC_2	106.5 B
C_2C_3	1.361 B	OC_2C_3	110.7 B
C_3C_4	1.431 A	$C_2C_3C_4$	106.0 B
C_2H	1.075 B	OC_2H	115.9 B
C_3H	1.077 A	C_4C_3H	127.9 A

[1] B. Bak, D. Christensen, W. B. Dixon, L. Hansen-Nygaard, J. R. Andersen, and M. Schottländer, J. Mol. Spectrosc. **9**, 124 (1962).

Thiophene

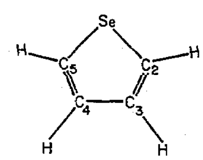


C_4H_4S C_{2v}

Bond	Substitution	Angle	Substitution
SC	1.714 B	CSC	92.1 A
C_1C_2	1.369 B	SC_1C_2	111.5 A
C_2C_2	1.423 B	$C_1C_2C_2$	112.5 A
C_1H	1.078 B	SCH	119.8 B
C_2H	1.080 B	C_2C_2H	124.3 A

[1] B. Bak, D. Christensen, L. Hansen-Nygaard and J. Rastrup-Andersen, J. Mol. Spectrosc. **7**, 58 (1961).
[2] B. Bak, D. Christensen, J. Rastrup-Andersen and E. Tannenbaum, J. Chem. Phys. **25**, 892 (1956).

Selenophene



C_4H_4Se C_{2v}

Bond	Substitution	Angle	Substitution
SeC_2	1.855 A	C_5SeC_2	87.8 B
C_2C_3	1.369 B	SeC_2C_3	111.6 B
C_3C_4	1.433 B	$C_2C_3C_4$	114.6 B
C_2H	1.070 B	SeC_2H_2	121.7 B
C_3H	1.079 B	$C_4C_3H_3$	122.9 B

[1] N. M. Posdeev, O. B. Akulinin, A. A. Shapkin and N. N. Magdesieva, J. Struct. Chem. **11**, 804 (1970).

1-Chloro-2-butyne

C_4H_5Cl $ClH_2C—C≡C—CH_3$ C_s

Bond	Effective	Angle	Effective
CH[a]	1.110[c]	HCH[a]	108.5[c]
CH[b]	1.090[c]	HCH[b]	108.5[c]
C≡C	1.207[c]	CCCl	111.5 X
CC[a]	1.458 X		
CC[b]	1.460 X		
CCl	1.798 X		

[a] Refers to CH_3 portion of molecule.
[b] Refers to CH_2Cl portion of molecule.
[c] These values were assumed.

[1] V. W. Laurie and D. R. Lide, J. Chem. Phys. **31**, 939 (1959).

Cyclopropanecarboxylic acid chloride

C_4H_5ClO $(C_3H_5)COCl$ C_s

The COCl group bisects the ring plane and has the Cl atom *cis* to the ring hydrogen.

[1] K. P. R. Nair and J. E. Boggs, J. Mol. Struct. **33**, 45 (1976).

Trifluoroacetic Acid-Acetic Acid Dimer

$C_4H_5F_3O_4$ $CF_3CO_2H \cdot CH_3CO_2H$

Bond	Effective
O···O	2.67 X

[1] C. C. Costain and G. P. Srivastava, J. Chem. Phys. **41**, 1620 (1964).

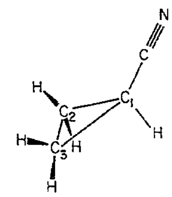
Butenonitrile
(Allyl Cyanide)

C_4H_5N $CH_2=CHCH_2CN$

Two rotational isomers, "*cis*" and "*gauche*" were identified. No further structural analyses were performed.

[1] K. V. L. N. Sastry, V. M. Rao and S. C. Dass, Can. J. Physics **46**, 959 (1968).

Cyclopropanecarbonitrile
(Cyclopropylcyanide)

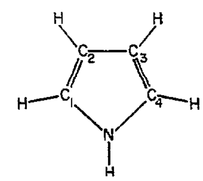


C_4H_5N C_s

Bond	Substitution	Angle	Substitution
C_1C_2	1.528 C	$C_2C_1C_3$	58.8 C
C_2C_3	1.500 A	$C_1C_2C_3$	60.6 C

[1] R. Pearson, Jr., A. Choplin and V. W. Laurie, J. Chem. Phys. **62** 4859 (1975).

Pyrrole

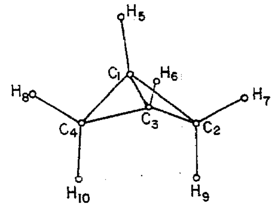


C_4H_5N C_{2v}

Bond	Substitution	Angle	Substitution
NC	1.370 B	CNC	109.8 B
C_1C_2	1.382 B	NCC	107.7 B
C_2C_3	1.417 B	CCC	107.4 B
NH	0.996 B	HC_2C_3	127.1 B
C_1H	1.076 B	HC_1C_2	130.7 B
C_2H	1.077 B		

[1] L. Nygaard, J. T. Nielsen, J. Kirchheiner, G. Maltesen, J. Rastrup-Andersen and G. O. Sorenson, J. Mol. Struct. **3**, 491 (1969).
[2] B. Bak, D. Christensen, L. Hansen and J. Rastrup-Andersen, J. Chem. Phys. **24**, 720 (1956).

Bicyclo[1.1.0]butane



C_4H_6			C_{2v}
Bond	Substitution	Angle	Substitution
C_1C_3	1.497 B	$C_1C_3C_2$	60.0 A
C_2C_3	1.498 B	$C_1C_2C_3$	60.0 A
C_2H_9	1.093 C	$C_2C_3C_4$	98.3 B
C_2H_7	1.093 C	HCH	115.6 B
C_1H_5	1.071 B	$H_9C_2C_3$	116.9 B
		$H_7C_2C_3$	118.1 B
		$C_2C_3H_6$	129.9 B
		$C_1C_3H_6$	128.4 B

The dihedral angle between the heavy atom planes is 121.7°.

[1] K. W. Cox and M. D. Harmony, J. Chem. Phys. **50**, 1976 (1969).
[2] M. D. Harmony and K. W. Cox, J. Amer. Chem. Soc. **88**, 5049 (1966).

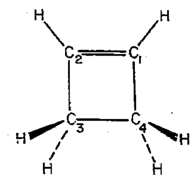
trans-1,3-Butadiene

C_4H_6	$C^1H_2{=}C^2HC^3H{=}C^4H_2$		C_{2h}
Bond	Effective	Angle	Effective
C^2C^3	1.464 X	$C^1C^2C^3$	123.2 X

Because of the assumptions required to derive the above structural parameters, the uncertainties are difficult to evaluate.

[1] A. R. H. Cole, G. M. Mohay and G. A. Osborne, Spectrochim. Acta **23A**, 909 (1967).
[2] D. J. Marais, N. Sheppard and B. P. Stoicheff, Tetrahedron **17**, 163 (1962).

Cyclobutene

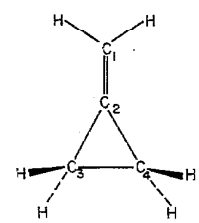


C_4H_6			C_{2v}
Bond	Substitution	Angle	Substitution
C_1C_2	1.342 B	$C_1C_2C_3$	94.2 B
C_1C_4	1.517 B	$C_2C_3C_4$	85.8 B
C_3C_4	1.566 B	HC_1C_2	133.5 B
C_1H	1.083 B	HC_3H	109.2 B
C_3H	1.094 B	HC_3C_4	114.5 B
		α[a]	135.8 B

[a] Angle between bisector of HCH and C_3C_4 bond.

[1] B. Bak, J. J. Led, L. Nygaard, J. Rastrup-Andersen and G. O. Sorensen, J. Mol. Struct. 3, 369 (1969).

Methylenecyclopropane

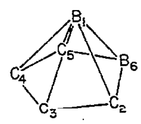


C_4H_6					C_{2v}
Bond	Substitution	Effective	Angle	Substitution	Effective
C_1C_2	1.332 B		$C_3C_2C_4$	63.9 B	
C_2C_3	1.457 B		HC_1H		114.3 D
C_3C_4	1.542 A		HC_3H		113.5 D
C_1H		1.088[a]	α[b]		29.2 D
C_3H		1.09 D			

Hydrogen parameters based upon assumed value of C_1H.
[a] Assumed value.
[b] Angle between HC_3H bisector and C_3C_4 bond axis.

[1] V. W. Laurie and W. M. Stigliani, J. Am. Chem. Soc. **92**, 1485 (1970).

2,3,4,5-Tetracarbahexaborane (6)



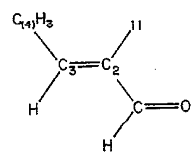
$C_4H_6B_2$ C_s

Bond	Substitution
B_1B_6	1.886 B
B_1C_2	1.709 E
B_1C_3	1.697 D
B_6C_2	1.541 C
C_2C_3	1.436 C
C_3C_4	1.424 C

Above structure was that obtained by choosing the positive sign for small C_2 (and C_5) *c* coordinates. The other choice leads to a less reasonable B_1C_2 distance.

[1] J. P. Pasinski and R. A. Beaudet, J. Chem. Phys. **61**, 683 (1974).

trans-2-Butenal (Crotonaldehyde)



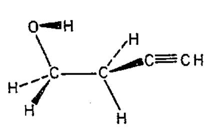
C_4H_6O C_s

Angle[a]	Effective
$C_2C_3C_4$	125.6 X
HC_3C_4	116.1 X

[a] Assumed values used for all other structural parameters.

[1] M. Suzuki and K. Kozima, Bull. Chem. Soc. Japan **42**, 2183 (1969).
[2] S. L. Hsu and W. H. Flygare, Chem. Phys. Lett. **4**, 317 (1969).

3–Butyn-1-ol

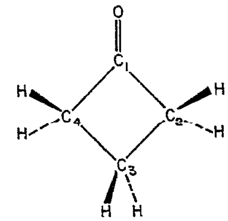


C_4H_6O C_1

Observed molecular conformation was *gauche*, with evidence for an intramolecular hydrogen bond.

[1] L. B. Szalanski and R. G. Ford, J. Mol. Spectrosc. **54**, 148 (1975).

Cyclobutanone



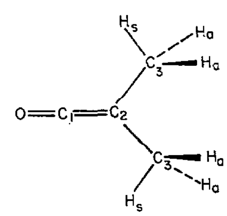
C_4H_6O C_{2v}

Bond	Substitution	Angle	Substitution
C_1C_2	1.529 B	$C_2C_1C_4$	93.0 B
C_2C_3	1.556 B	$C_1C_2C_3$	88.1 B
CO	1.204 C	$C_2C_3C_4$	90.8 B
C_2H	1.099 B	HC_2H	109.2 C

The HC_2H group is tilted toward the carbonyl group by 4.6° (C).

[1] W. M. Stigliani and V. W. Laurie, J. Mol. Spectrosc. **62**, 85 (1976).
[2] L. H. Scharpen and V. M. Laurie, J. Chem. Phys. **49**, 221 (1968).

Dimethylketene



C_4H_6O C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
CH_s	1.088 C		$C_1C_2C_3$		120.6 X
CH_a	1.093 B		CCH_s		111.5 X
CO		1.171	CCH_a		110.6 X
C_1C_2		1.300 X	H_aCH_a	107.3 C	
C_2C_3		1.514 X	H_sCH_a	108.3 C	

CO bond length was fixed at value reported for ketene.

[1] K. P. R. Nair, H. D. Rudolph, and H. Dreizler, J. Mol. Spectrosc. **48**, 571 (1973).

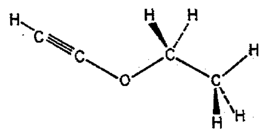
3,4-Epoxy-1-butene

C_4H_6O $H_2C{=}CH{-}CH{-}O{-}CH_2$ (ring: CH and CH_2 bonded) C_1

The molecule was shown to exist in the *trans* conformation relative to the CC single bond.

[1] T. Ikeda, K. V. L. N. Sastry and R. F. Curl, Jr., J. Mol. Spectrosc. **56**, 411 (1975).

Ethoxyethyne



C_4H_6O C_s

The spectrum of the *anti* conformation, shown above, is consistent with a planar heavy-atom skeleton. A less stable *gauche* form, having a dihedral angle about the CO bond of 108° (X), was also observed.

[1] A. Bjorseth, J. Mol. Struct. **20**, 61 (1974).

3-Methoxy-1-propyne (Methylpropargyl ether)

C_4H_6O $CH_3—O—CH_2—C≡CH$ C_1

The observed stable molecular conformation was *gauche* with respect to the CO bond, the reported dihedral angle being 68° (0° = *syn* conformation).

[1] K. M. Marstokk and H. Mollendal, J. Mol. Struct. **32**, 191 (1976).

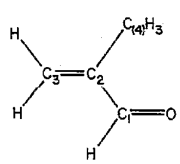
3-Methyleneoxetane

C_4H_6O $H_2C=C—CH_2—O—CH_2$ (ring) C_{2v}

Analysis of ground and excited states of the ring-puckering vibration indicated a planar heavy-atom equilibrium structure.

[1] J. S. Gibson and D. O. Harris, J. Chem. Phys. **52**, 5234 (1970).

trans-2-Methyl-2-propenal



C_4H_6O C_s

Angle[a]	Effective
$C_3C_2C_4$	123.4 X
$C_1C_2C_3$	116.4 X

[a] Assumed values used for all other structural parameters.

[1] M. Suzuki and K. Kozima, J. Mol. Spectrosc. **38**, 314 (1971).

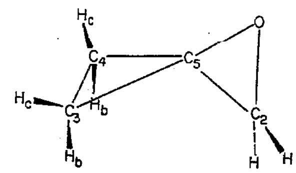
Methyl vinyl ketone

C_4H_6O $H_3C—CO—CH=CH_2$ C_s

Observed conformation is that with the carbonyl *trans* to the vinyl group.

[1] P. D. Foster, V. M. Rao and R. F. Curl, Jr., J. Chem. Phys. **43**, 1064 (1965).

Oxaspiro[2.2]pentane

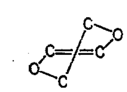


C_4H_6O C_s

Bond	Substitution	Angle	Substitution
C_2O	1.460 B	HC_2H	117.0 B
C_3C_4	1.550 B	HC_3H	115.0 C
C_3C_5	1.470 C	C_2OC_5	60.4 B
C_5O	1.416 C	C_2C_5O	61.3 C
C_2C_5	1.447 C	$C_3C_5C_4$	63.6 C
C_2H	1.086 B	$C_5C_3C_4$	58.2 C
C_3H_b	1.080 C	HC_2C_5	119.5 B
C_3H_c	1.075 C	HC_2O	114.1 B
		$H_bC_3H_5$	118.9 C
		$H_bC_3C_4$	116.9 B
		$H_cC_3C_5$	118.0 C
		$H_cC_3C_4$	116.9 B

[1] W. D. Slafer, A. D. English, D. O. Harris, D. F. Shellhamer, M. J. Meshishnek and D. H. Aue, J. Am. Chem. Soc. **97**, 6638 (1975).

2,3-Dihydro-*p*-dioxin (1,4-Dioxene)



$C_4H_6O_2$ C_2

The twist (half-chair) conformation was reliably established.

[1] J. A. Wells and T. B. Malloy, Jr., J. Chem. Phys. **60**, 2132 (1974).

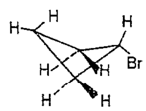
Ethylthioethyne

C_4H_6S	$(CH_3CH_2)S(C{\equiv}CH)$	C_1

The observed spectrum was consistent only with the methyl group occupying a *gauche* conformation, 119° (X) from the *anti* position.

[1] A. Bjorseth, J. Mol. Struct. **23**, 1 (1974).

Bromocyclobutane

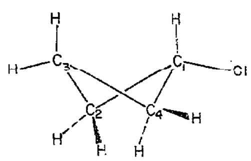


C_4H_7Br	$\overline{CH_2CH_2CH_2CHBr}$	C_s

Ring is puckered with a dihedral angle of approximately 29°. Only the equatorial form was observed.

[1] W. G. Rothschild and B. P. Dailey, J. Chem. Phys. **36**, 2931 (1962).

Chlorocyclobutane



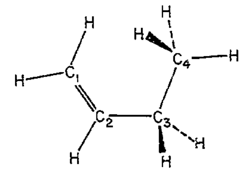
C_4H_7Cl C_s

Bond	Effective	Angle	Effective
C_1Cl	1.775 D	HCCl	114 D
C_1C_2	1.525 D	$C_2C_1C_4$	91 D
C_2C_3	1.550 D	HC_2H	112 D
C_1H	1.10 D	HC_3H	110 D
C_2H	1.09 D	HC_2C_1	114 D
C_3H	1.10 D		
		ring dihedral	20 D
		CCl with $C_2C_1C_4$ plane	135 D

CH_2 groups were assumed to bisect ring angles. Only equatorial Cl observed.

[1] H. Kim and W. D. Gwinn, J. Chem. Phys. **44**, 865 (1966).

cis-1-Butene



C_4H_8 C_s

Bond	Effective	Angle	Effective
C_1C_2	1.336 D	$C_1C_2C_3$	126.7 D
C_2C_3	1.507 D	$C_2C_3C_4$	114.8 D
C_3C_4	1.536 D	HC_2C_3	115.1 D
		HC_4C_3	110.4 D
		HC_3H	105.2 D

CH bond lengths were assumed. HC_3H was assumed to bisect $C_2C_3C_4$. The *skew* form was also observed. See the following.

[1] S. Kondo, E. Hirota, Y. Morino, J. Mol. Spectrosc. **28**, 471 (1968).

skew-1-Butene

C_4H_8	$C^1H_2{=}C^2HC^3H_2C^4H_3$	C_1

Bond	Effective	Angle	Effective
C^1C^2	1.342 D	$C^1C^2C^3$	125.4 C
C^2C^3	1.493 D	$C^2C^3C^4$	112.1 C
C^2C^4	1.536 D	dihedral[a]	119.9 C
		HC^2C^3	117.1 E
		HC^4C^3	110.3 D
		HC^3H	105.7 D

CH bond lengths were assumed. The *cis* form was also observed. See the preceding.

[a] Angle between $C_1C_2C_3$ and $C_2C_3C_4$ planes.

[1] S. Kondo, E. Hirota, and Y. Morino, J. Mol. Spectrosc. **28**, 471 (1968).

cis-2-Butene

C_4H_8	$H_3CCH{=}CHCH_3$	C_{2v}

Bond	Effective	Angle	Effective
CC	1.497 D	CCC	126.7 D

A number of structural parameters were assumed.

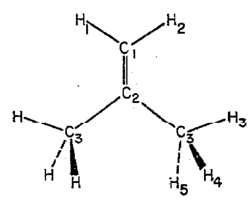
[1] S. Koudo, Y. Sakurai, E. Hirota, and Y. Morino, J. Mol. Spectrosc. **34**, 231 (1970).

Cyclobutane

C_4H_8	$CH_2CH_2CH_2CH_2$ (ring)		D_{2d}
Bond	Effective	Angle	Effective
CC	1.558 C	ring dihedral	35 E

[1] R. C. Lord and B. P. Stoicheff, Can. J. Phys. **40**, 725 (1962).
[2] J. M. R. Stone and I. M. Mills, Mol. Phys. **18**, 631 (1970).
[3] F. A. Miller and R. J. Capwell, Spectrochim. Acta **27A**, 947 (1971).

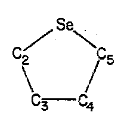
2-Methylpropene (Isobutylene)



C_4H_8			C_{2v}
Bond	Substitution	Angle	Substitution
C_1C_2	1.330 D	$C_1C_2C_3$	115.3 D
C_2C_3	1.507 C	$H_1C_1H_2$	118.5 B
C_1H_1	1.088 B	$C_2C_3H_3$	112.9 E
C_3H_3	1.072 E	$C_2C_3H_4$	110.7 C
C_3H_4	1.095 C	$H_4C_3H_5$	106.0 C

[1] L. H. Scharpen and V. W. Laurie, J. Chem. Phys. **39**, 1732 (1963).
[2] V. W. Laurie, J. Chem. Phys. **34**, 1516 (1961).

Tetrahydroselenophene



C_4H_8Se			C_2
Bond	Substitution	Angle	Substitution
SeC_2	1.963 B	C_2SeC_5	90.7 B
C_2C_3	1.549 B	SeC_2C_3	104.0 B
C_3C_4	1.527 B	$C_2C_3C_4$	106.9 C
		α[a]	29.7 C

[a] Twist angle formed by intersection of C_5SeC_2 plane and C_4SeC_3 plane.

[1] A. H. Mamleev, N. M. Pozdeev and N. N. Magdesieva, J. Mol. Struct. **33**, 211 (1976).

2-Chloro-2-methylpropane (Tertiary butyl chloride)

C_4H_9Cl		$(CH_3)_3CCl$			C_{3v}
Bond	Substitution	Average	Angle	Substitution	Average
CCl	1.803 B	1.831 D	CCCl	108.0 B	107.0 C
CC	1.530 B	1.525 B			

Bond	Effective	Angle	Effective
CCl	1.828 B	CCCl	111.7 D
CC	1.528 B	HCH	109.4 B
CH	1.097 B		

[1] D. R. Lide and M. Jen, J. Chem. Phys. **38**, 1504 (1963).
[2] R. L. Hilderbrandt and J. D. Wieser, J. Chem. Phys. **56**, 1143 (1972).
[3] W. Braun, H. Günther, H. Umbrecht and W. Zeil, Z. Physik. Chem. **93**, 247 (1974).

2-Fluoro-2-methylpropane (Tertiary Butyl Fluoride)

C_4H_9F	$(CH_3)_3CF$		C_{3v}
Bond	Effective	Angle	Effective
CF	1.43 D	CCC	112.7 C
CC	1.516 C	HCH	107.9 D

CH distance was fixed at 1.090 Å.

[1] D. R. Lide and D. E. Mann, J. Chem. Phys. **29**, 914 (1958).

Trimethylgermanecarbonitrile (Trimethylcyanogermane)

C_4H_9GeN		$(CH_3)_3GeCN$		C_{3v}
Bond	Substitution	Effective	Angle	Effective
CN	1.115 A		CGeC(N)	106.2 X
GeC(N)	1.947 C		HCGe	111.0[a]
GeC(H_3)		1.930 X		
CH		1.095[a]		

[a] Assumed values.

[1] J. R. Durig, Y. S. Li and J. B. Turner, Inorg. Chem. **13**, 1495 (1974).

2-Iodo-2-methylpropane (Tertiary butyl iodide)

C_4H_9I $(CH_3)_3CI$ C_{3v}

Bond	Effective	Angle	Effective
CI	2.190 C	CCC	111.0 A
CC	1.527 B		

The parameters CC, CH and CCC were assumed to obtain CI.

[1] J. Q. Williams and W. Gordy, J. Chem. Phys. **18**, 994 (1950).
[2] W. Winkle and H. Hartmann, Z. Naturforsch. **25a**, 840 (1970).

Trimethylsilyl isocyanate

C_4H_9NOSi $(CH_3)_3SiNCO$ C_{3v}

The spectral evidence is consistent with a linear or very nearly linear Si—N=C=O group.

[1] A. J. Careless, M. C. Green and H. W. Kroto, Chem. Phys. Lett. **16**, 414 (1972).

Trimethylsilylcyanide

C_4H_9NSi $(CH_3)_3SiCN$ C_{3v}

The conventionally prepared sample of this compound was found to contain (based upon symmetric rotor spectra for each isomer) approximately 5% of the isocyanide (—SiNC) isomer.

[1] J. R. Durig, W. O. George, Y. S. Li and R. O. Carter, J. Mol. Struct. **16**, 47 (1973).

2-Methyl propane (Isobutane)

C_4H_{10} $(CH_3)_3CH$ C_{3v}

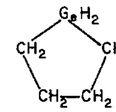
Bond	Substitution	Average	Angle	Substitution
CC	1.525 B	1.532 B	CCC	111.2 B
CH_t	1.108 B	1.109 B	CCH_s	109.4 C
CH_s	1.100 D	1.083 C	H_aCH_a[a]	108.5 D
CH_a	1.092[a] D	1.083 C	H_aCH_s[a]	107.9 D

Average structure parameters are r_z values from combined microwave-electron diffraction data. H_t refers to tertiary hydrogen, and H_s and H_a refer to the in-plane and out-of-plane atoms, respectively.

[a] These parameters utilized assumption that methyl hydrogens form an equilateral triangle.

[1] D. R. Lide, J. Chem. Phys. **33**, 1519 (1960).
[2] R. L. Hilderbrandt and J. D. Wieser, J. Mol. Struct. **15**, 27 (1973).

Germacyclopentane



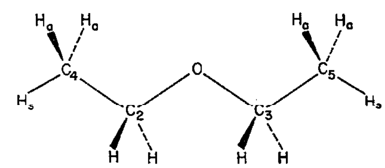
$C_4H_{10}Ge$ C_2

Angle[a]	Effective
CGeC	98° X
CCGe	106° X
CCC	115° X
Twist	18° X

[a] Determined by fitting moments of inertia along with the assumptions CGe = 1.95A, CC = 1.53A, CH = 1.09A, GeH = 1.53A, HCH = 109°, HGeH = 111°.

[1] E. C. Thomas and V. W. Laurie, J. Chem. Phys. **51**, 4327 (1969).

Diethyl ether



$C_4H_{10}O$ C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
CO	1.408 B		COC	112.6 B	
CC	1.516 B		OCC	108.6 B	
C_2H	1.100 B		C_4C_2H	110.4 B	
C_4H_a	1.090 B				
C_4H_s		1.090 X	OC_2H	109.9 B	
			$C_2C_4H_a$	110.2 B	
			$C_2C_4H_s$		110.6 D
			$H_aC_4H_a$	108.1 C	
			$H_sC_4H_a$		108.6 C

The b coordinate of H_s was computed under the assumption that C_4H_a = C_4H_s. The coordinates of the methylene H atoms were recomputed from the reported rotational constants.

[1] M. Hayashi and K. Kuwada, Bull. Chem. Soc. Japan **47**, 3006, 1974.
[2] M. Hayashi and K. Kuwada, Bull. Chem. Soc. Japan **44**, 299 (1971).

Methylpropyl ether

$C_4H_{10}O$ $(CH_3)O(C_3H_7)$ C_s

The observed spectrum is consistent only with the *trans-trans* conformation.

[1] M. Hayashi, M. Imachi, J. Nakagawa and A. Ozaki, Chem. Lett. (Japan) **1977**, 41 (1977).

C_5–C_{11} Molecules

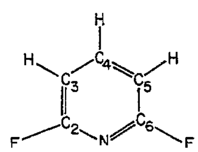
Cyanobutadiyne (Cyanodiacetylene)

C_5HN $H—C^1≡C^2—C^3≡C^4—C^5≡N$ $C_{\infty v}$

Bond	Substitution
CH	1.057 B
C^1C^2	1.209 A
C^2C^3	1.362 B
C^3C^4	1.222 B
C^4C^5	1.364 B
C^5N	1.161 A

[1] A. J. Alexander, H. W. Kroto and D. R. M. Walter, J. Mol. Spectrosc. **62**, 175 (1976).

2,6-Difluoropyridine

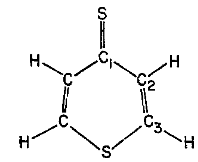


$C_5H_3F_2N$ C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
NC_2	1.317 B		$C_3C_4C_5$	119.8 A	
C_2C_3	1.377 C		$C_2C_3C_4$	116.1 A	
C_3C_4	1.394 A		NC_2C_3	126.5 B	
C_3H	1.080 B		C_2NC_6	115.0 B	
C_4H	1.082 B		C_3C_4H	120.1 B	
C_2F		1.347 B	C_2C_3H	120.8 B	
			C_3C_2F		118.8 B

[1] O. L. Stiefvater, Z. Naturforsch. **30a**, 1765 (1975).

4H-Thiapyran-4-thione



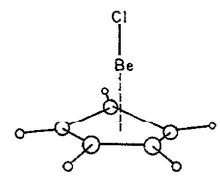
$C_5H_4S_2$ C_{2v}

Bond	Substitution	Angle	Substitution
C_1S	1.671 B	$C_2C_1C_2$	117.5 D
C_3S	1.759 A	$C_1C_2C_3$	128.1 D
C_1C_2	1.406[a] D	C_2C_3S	122.4 C
C_2C_3	1.342[a] D	C_3SC_3	101.4 A

[a] These parameters required that hydrogen positions be fixed by assumption.

[1] M. J. Corkill, A. P. Cox and I. C. Ewart, J. C. S. Chem. Comm. **1976**, 546 (1976).

Cyclopentadienylberyllium chloride



C_5H_5BeCl C_{5v}

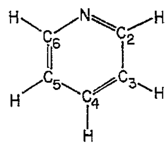
Bond	Substitituon	Effective
CC	1.424 B	1.424 B
BeCl	1.81 E	1.839 C
h[a]	1.52 E	1.485 C
CH	1.09 E	1.090 D
Cl···C	3.546 B	3.538 B

Hydrogen atoms were assumed to be coplanar with the five-membered ring. Also, to obtain CH substitution distance, the value B − C = 26.8 MHz was assumed for the monodeuterated species.

[a] Distance of Be atom from plane of the five-membered ring.

[1] A. Bjorseth, D. A. Drew, K. M. Marstokk and H. Mollendal, J. Mol. Struct. **13**, 233 (1972).

Pyridine

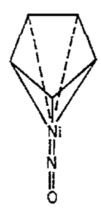


C_5H_5N — C_{2v}

Bond	Substitution	Angle	Substitution
NC_2	1.338 A	C_6NC_2	116.9 A
C_2C_3	1.394 B	NC_2C_3	123.8 A
C_3C_4	1.392 A	$C_2C_3C_4$	118.5 A
C_2H	1.086 B	$C_3C_4C_5$	118.4 A
C_3H	1.082 B	NC_2H	116.0 B
C_4H	1.081 B	C_2C_3H	120.1 B
		C_3C_4H	120.8 B

[1] G. O. Sorensen, L. Mahler and N. Rastrup-Andersen, J. Mol. Struct. **20**, 119 (1974).
[2] B. Bak, L. Hansen-Nygaard and J. Rastrup-Andersen, J. Mol. Spectrosc. **2**, 361 (1958).

π-Cyclopentadienylnitrosylnickel



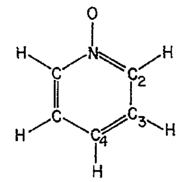
C_5H_5NNiO — C_{5v}

Bond	Substitution	Effective
NO	1.165 B	
NiN	1.626 C	
NiC		2.11 C
CC		1.43 C

No information regarding the planarity of the C_5H_5 ring system (i.e., coplanarity of C_5, H_5 planes) was obtained. The CH distances were assumed.

[1] A. P. Cox and A. H. Brittain, Trans. Faraday Soc. **66**, 557 (1970).

Pyridine N-oxide



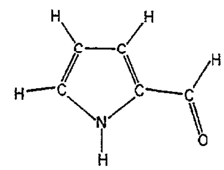
C_5H_5NO — C_{2v}

Bond	Substitution	Effective	Angle	Substitution
NC_2	1.362 C		CNC	119.8 C
C_2C_3	1.389 C		NCC	120.7 B
C_3C_4	1.395 A		$C_2C_3C_4$	120.6 A
NO		1.278 D	$C_3C_4C_5$	117.6 A

Hydrogen parameters were assumed to obtain the NO distance.

[1] O. Snerling, C. J. Nielsen, L. Nygaard, E. J. Pedersen and G. O. Sorensen, J. Mol. Struc. **27**, 205 (1975).

cis-Pyrrole-2-carboxaldehyde



C_5H_5NO — C_s

The *cis* conformation was definitely established with a non-bonding O ··· H distance of 2.592 (C).

[1] K. M. Marstokk and H. Mollendal, J. Mol. Struct. **23**, 93 (1974).

Cyclopentadienyl Thallium

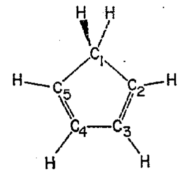
C_5H_5Tl — C_{5v}

Bond	Effective
CC	1.43 X
CTl	2.705 X

C_5H_5 moiety was assumed to be coplanar, with CH = 1.080 Å.

[1] J. K. Tyler, A. P. Cox and J. Sheridan, Nature **183**, 1182 (1959).

Cyclopentadiene



C_5H_6 C_{2v}

Bond	Substitution	Angle	Substitution
C_1C_2	1.506 B	$C_5C_1C_2$	102.9 B
C_2C_3	1.344 B	$C_1C_2C_3$	109.2 B
C_3C_4	1.468 B	$C_2C_3C_4$	109.3 B
C_1H	1.099 B	HC_1H	106.3 B
C_2H	1.078 B	HC_2C_3	127.1 B
C_3H	1.080 B	HC_3C_2	126.0 B

[1] D. Damiani, L. Ferretti and E. Gallinella, Chem. Phys. Lett. 37, 265 (1976).
[2] L. H. Scharpen and V. W. Laurie, J. Chem. Phys. 43, 2765 (1965).

3-Pyridinamine (3-Aminopyridine)

$C_5H_6N_2$ CH—CH—CH—N—CH—C—NH$_2$ (ring) C_1

Bond	Substitution	Angle	Effective
H ··· H′	1.672 E	HNH′	113.4 E
		ϕ	37.0 X

The parameters for the amine group are obtained from the deuterium substitution along with the assumption that d (NH) = 1.00 A and some assumptions for ring parameters. ϕ is the angle between the HNH bisector and the CN bond.

[1] D. Christen, D. Norbury, D. G. Lister and P. Palmieri, J.C.S., Faraday II, 1975, 438.

4-Pyridinamine (4-Aminopyridine)

$C_5H_6N_2$ CH—CH—N—CH—CH—C—NH$_2$ (ring) C_s

Bond	Substitution	Angle	Effective
H ··· H′	1.699 E	HNH′	116.3 E
		ϕ	27.6 X

The parameters for the amine group are obtained from deuterium substitution data along with the assumption that d(NH) = 1.00 A and some assumptions for ring parameters. ϕ is the angle between the HNH bisector and the CN bond.

[1] D. Christen, D. Norbury, D. G. Lister and P. Palmieri, J.C.S., Faraday II, 1975, 438.

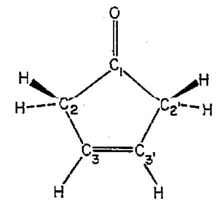
Cyclopent-2-en-1-one

C_5H_6O CH$_2$CH$_2$CH=CHC=O (ring) C_s

Planarity of heavy atoms has been conclusively established.

[1] D. Chadwick, A. C. Legon and D. J. Millen, Chem. Comm. 1969, 1130 (1969).

Cyclopent-3-en-1-one



C_5H_6O C_{2v}

Bond	Substitution	Angle	Substitution
CO	1.210 A	$C_2C_1C_{2'}$	109.2 C
C_1C_2	1.524 C	$C_1C_2C_3$	103.1 C
C_2C_3	1.509 C	$C_2C_3C_{3'}$	112.4 B
$C_3C_{3'}$	1.338 B	HC_2H	107.3 C
C_2H	1.086 B	HC_3C_2	124.7 B
C_3H	1.079 B	θ^a	0.0 C

[a] Angle between the bisectors of the HC_2H and $C_1C_2C_3$ angles.

[1] J. W. Bevan and A. C. Legon, J. Chem. Soc. Faraday Trans., 67, 902 (1973).

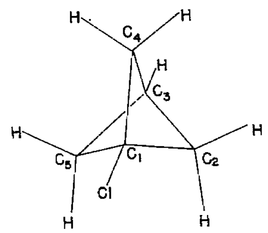
2-Methylfuran

C_5H_6O C_s

Heavy atom planarity seems assured by the data. See structure of furan.

[1] U. Andersen and H. Dreizler, Z. Naturforsch. 25a, 570 (1970).
[2] W. G. Norris and L. C. Krisher, J. Chem. Phys. 51, 403 (1969).

1-Chlorobicyclo[1.1.1]Pentane



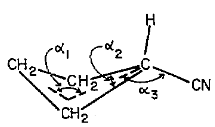
C_5H_7Cl C_{3v}

Bond	Effective	Angle	Effective
C_1C_2	1.536 X	$C_1C_2C_3$	73.5 X
C_2C_3	1.556 X	$C_2C_1C_4$	88.6 X
C_1Cl	1.761 X	$C_2C_3C_4$	87.2 X
		ClC_1C_2	126.2 X

In order to obtain the structural parameters, the constraint $r(C_2C_3)-r(C_1C_2) = 0.02 \pm 0.01$ Å and parameters for the methylene groups had to be assumed.

[1] K. W. Cox and M. D. Harmony, J. Mol. Spectrosc. 36, 34 (1970).

Cyclobutanecarbonitrile



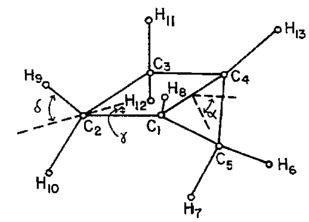
C_5H_7N C_s

Angle	Effective
α_1	21.4 X
α_2	90.0 X
α_3	133.0 X

The equatorial conformation was established.

[1] M. Y. Fong and M. D. Harmony, J. Chem. Phys. 58, 4260 (1973).

Bicyclo[2.1.0]pentane



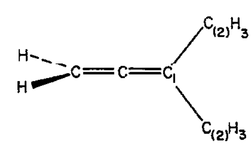
C_5H_8 C_s

Bond	Substitution	Angle	Substitution
C_1C_4	1.536 B	$C_1C_2H_9$	113.3 D
C_2C_3	1.565 B	$C_1C_2H_{10}$	115.2 C
C_1C_2	1.528 C	$C_3C_2H_9$	111.9 C
C_1C_5	1.507 B	$C_3C_2H_{10}$	116.6 D
C_5H_6	1.088 B	$H_6C_5H_7$	116.7 C
C_5H_7	1.090 B	$H_8C_1C_5$	121.2 C
C_1H_8	1.082 B	$H_8C_1C_4$	128.6 C
C_2H_9	1.085 C	α	67.3 C
C_2H_{10}	1.097 C	β	61.0 C

Redundant parameters: $H_6C_5C_1$ = 114.7 (C), $H_7C_5C_1$ = 119.0 (B), $H_8C_1C_2$ = 126.3 (C), $H_9C_2H_{10}$ = 109.4 (C), γ = 44.8 (C), δ = 57.3 (D). Angle β is the acute angle formed by the intersection of C_5H_6 with the bisector of the $C_1C_5C_4$ angle.

[1] S. N. Mathur, M. D. Harmony and R. D. Suenram, J. Chem. Phys. 64, 4340 (1976).

Dimethylallene



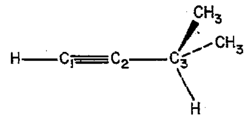
C_5H_8 C_{2v}

Bond	Effective	Angle	Effective
$C_1C_{(2)}$	1.514 X	$C_{(2)}C_1C_{(2)}$	116.4 X

Double-bond distances were fixed at the allene value, 1.308 Å; methyl group and vinyl hydrogen parameters were taken from dimethyl ketene and allene structures, respectively.

[1] J. Demaison and H. D. Rudolph, J. Mol. Spectrosc. 40, 445 (1971).

3-Methyl-1-butyne



C_5H_8 C_s

Bond	Effective	Angle	Effective
$C_{Me}C_3$	1.527 X	$C_{Me}C_3C_2$	109.6 X
C_2C_3	1.495 X	$C_{Me}CC_{Me}$	112.9 X
C_1C_2[a]	1.203 A	HC_1C_2[a]	180.0
C_1H[a]	1.058 A	$HC_{Me}H$[a]	109.5
$C_{Me}H$[a]	1.092		

[a] Assumed value.

[1] A. R. Mochel, A. Bjørseth, C. O. Britt, and J. E. Boggs, J. Mol. Spectrosc. 48, 107 (1973).

Cyclopentanone

C_5H_8O $\overline{CH_2CH_2CH_2CH_2C}$=O C_2

The ground state conformation is a twisted C_2 form.

[1] H. Kim and W. D. Gwinn, J. Chem. Phys. 51, 1815 (1969).

Pivalonitrile (Tertiary Butyl Cyanide)

C_5H_9N $(C^1H_3)_3C^2C^3N$ C_{3v}

Bond	Substitution	Angle	Substitution
C^3N	1.159 A	$C^1C^2C^1$	110.5 C
C^1C^2	1.536 C		
C^2C^3	1.478 C		

[1] L. J. Nugent, D. E. Mann and D. R. Lide, J. Chem. Phys. 36, 965 (1962).

Cyclopentane

C_5H_{10} $\overline{CH_2CH_2CH_2CH_2CH_2}$ Undetermined

Bond	Effective
CC	1.537 X

D_{5h} symmetry was assumed in the derivation of the above bond distance.

[1] K. Tanner and A. Weber, J. Mol. Spectrosc. 10, 381 (1963).

1,3,5-Trifluorobenzene

$C_6H_3F_3$ D_{3h}

Bond	Effective
CF	1.304 X

In order to determine r_0(C—F) the CC and CH bond distances were assumed.

[1] J. Schlupf and A. Weber, J. Raman Spectrosc. 1, 3 (1973).

1-Chloro-2-fluorobenzene (o-Fluorochlorobenzene)

C_6H_4ClF C_s

Bond	Effective
CC	1.397 X
CH	1.084 X
CF	1.31 X
CCl	1.72 X

Structure assumes ring is a regular hexagon.

[1] P. Kökeritz and H. Selen, Ark. Fys. 30, 193 (1965).

1-Chloro-3-fluorobenzene (*m*-Fluorochlorobenzene)

C_6H_4ClF C_s

Bond	Effective
CC	1.397 X
CH	1.084 X
CF	1.329 X
CCl	1.699 X

Structure assumes ring is a regular hexagon.

[1] A. Rachman, P. Kökeritz and H. Selen J. Mol. Spectrosc. 8, 338 (1962).

m-Difluorobenzene (1,3-Difluorobenzene)

$C_6H_4F_2$ C_{2v}

Bond	Effective
CC	1.40 X
CH	1.084 X
CF	1.30 X

Ring assumed to be regular hexagon.

[1] L. Nygaard, E. R. Hansen, R. L. Hansen, J. Rastrup-Andersen, and G. O. Sorensen, Spectrochim. Acta 23A, 2813 (1967).

o-Difluorobenzene (1,2-Difluorobenzene)

$C_6H_4F_2$ C_{2v}

Bond	Effective
CC	1.40 X
CH	1.084 X
CF	1.31 X

Ring assumed to be regular hexagon.

[1] A. Hatta, C. Hirose, and K. Kozima, Bull. Chem. Soc. Japan **41**, 1088 (1968).
[2] L. Nygaard, E. R. Hansen, R. Lykke. Hansen, J. Rastrup-Andersen and G. O. Sorensen, Spectrochim. Acta **23A**, 2813 (1967).

o-Benzoquinone

$C_6H_4O_2$ O—C—CH═CH—CH═CH C═O C_{2v}

The observed microwave spectrum supports a planar molecule with the quinonoid structure.

[1] G. L. Blackman, R. D. Brown and A. P. Porter, J. C. S. Chem. Comm. **1975**, 499 (1975).

Bromobenzene

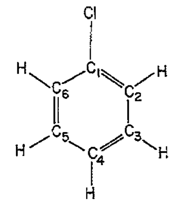
C_6H_5Br C_{2v}

Bond	Effective
CC	1.40 X
CH	1.07 X
CBr	1.87 X

Structure assumes regular hexagon. Four isotopic species studied (no C^{13} species).

[1] E. Rosenthal and B. P. Dailey, J. Chem. Phys. **43**, 2093 (1965).

Chlorobenzene

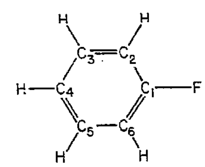


C_6H_5Cl C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
C_1C_2	1.399 B	1.402 B	$C_6C_1C_2$	120.2 B	120.2 B
C_2C_3	1.386 C	1.390 C	$C_1C_2C_3$	119.8 B	119.7 B
C_3C_4	1.398 A	1.398 A	$C_2C_3C_4$	120.2 A	120.2 A
C_1Cl	1.725 B	1.722 B	$C_3C_4C_5$	119.8 A	120.0 A
C_2H	1.080 C	1.077 C	ClC_1C_2	119.9 B	119.9 B
C_3H	1.081 B	1.079 B	C_1C_2H	119.5 C	119.5 C
C_4H	1.081 B	1.080 B	C_2C_3H	119.8 B	119.6 B
			C_3C_4H	120.1 A	120.0 A

[1] F. Michel, H. Nery, P. Nosberger, and G. Roussy, J. Mol. Struct. **30**, 409 (1976).
[2] G. Roussy and F. Michel, J. Mol. Struct. **30**, 399 (1976).

Fluorobenzene



C_6H_5F C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
C_1C_2		1.383 D	$C_6C_1C_2$		123.4 D
C_2C_3		1.395 D	$C_1C_2C_3$		117.9 D
C_3C_4	1.397 B		$C_2C_3C_4$		120.5 D
C_1F		1.354 D	$C_3C_4C_5$	119.8 B	
C_2H		1.081 D	C_1C_2H		120.0 D
C_3H	1.083 C		C_4C_3H	119.9 C	
C_4H	1.080 C				

[1] B. Bak, D. Christensen, L. Hansen-Nygaard, and E. Tannenbaum, J. Chem. Phys. **26**, 134 (1957).
[2] L. Nygaard, I. Bojesen, T. Pederson, and J. Rastrup-Andersen, J. Mol. Struct. **2**, 209 (1968).

Iodobenzene

C_6H_5I C_{2v}

Bond	Effective
CC	1.397 X
CH	1.084 X
CI	2.08 X

Structure assumes ring is a regular hexagon.

[1] K. Johansson, H. Oldeberg and H. Selen, Ark. Fys. **29**, 531 (1965).

Nitrosobenzene

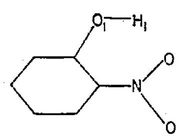
C_6H_5NO C_s

Bond	Effective	Angle	Effective
CN	1.47 X	CNO	116 X

Ring parameters were taken to be those of benzonitrile and NO distance was chosen to be 1.21.

[1] Y. Hanyu and J. E. Boggs, J. Chem. Phys. **43**, 3454 (1965).

2-Nitrophenol



$C_6H_5NO_3$ C_s

Bond	Substitution
O_1H_1	1.00 D

[1] S. Leavell and R. F. Curl, Jr., J. Mol. Spectrosc. **45**, 428 (1973).

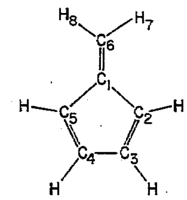
Benzene

C_6H_6 D_{6h}

Bond	Effective
CC	1.396 B
CH	1.083 B

[1] A. Cabana, J. Bachand and J. Giguere, Can. J. Phys. **52**, 1949 (1974).

5-Methylene-1,3-Cyclopentadiene (Fulvene)

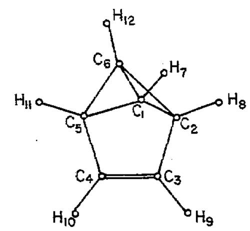


C_6H_6 C_{2v}

Bond	Substitution	Angle	Substitution
C_1C_6	1.348 A	$C_2C_1C_5$	106.8 A
C_1C_2	1.468 A	$C_1C_2C_3$	107.7 A
C_2C_3	1.357 A	$C_2C_3C_4$	108.9 A
C_3C_4	1.476 A	C_1C_2H	124.9 A
C_2H	1.077 A	C_2C_3H	126.4 A
C_3H	1.080 A	$H_7C_6H_8$	118.1 A
C_6H_7	1.083 A		

[1] P. A. Baron, R. D. Brown, F. R. Burden, P. J. Domaille and J. E. Kent, J. Mol. Spectrosc. **43**, 401 (1972).
[2] R. D. Suenram and M. D. Harmony, J. Chem. Phys. **58**, 5843 (1973).

Tricyclo[3.1.0.0^{2,6}]hex-3-ene (Benzvalene)



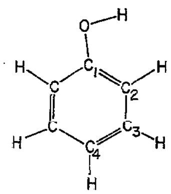
C_6H_6 C_{2v}

Bond	Substitution	Angle	Substitution
C_1C_6	1.452 A	α^a	106.0 C
C_1C_2	1.529 B	$C_6C_1H_7$	133.7 A
C_2C_3	1.503 C	$C_2C_1H_7$	135.3 A
C_3C_4	1.339 A	$C_1C_2H_8$	119.8 C
C_1H_7	1.078 A	$C_3C_2H_8$	124.2 C
C_2H_8	1.082 A	$C_2C_3H_9$	125.4 A
C_3H_9	1.078 A	$C_4C_3H_9$	128.9 A
		$C_2C_3C_4$	105.7 A

[a] Dihedral angle of four membered ring.

[1] R. D. Suenram and M. D. Harmony, J. Amer. Chem. Soc. **95**, 4506 (1973).

Phenol



C_6H_6O C_s

Bond	Effective	Substitution	Angle	Effective
CC	1.397 X		COH	109.0 X
C_2H	1.084 X		OC_1C_2	122.2 X
C_3H	1.076 X			
C_4H	1.082 X			
CO	1.364 X			
OH		0.956 X		

Assumed:
Ring is a regular hexagon.
C_2 axis of benzene ring coincides with the *b* principal axis.
Center of mass of OH group lies on the *b* axis.

[1] T. Kojima, J. Phys. Soc. Japan **15**, 284 (1960).
[2] H. Forest and B. P. Dailey, J. Chem. Phys. **45**, 1736 (1966).
[3] T. Pederson, M. W. Larsen and L. Nygaard, J. Mol. Struct. **4**, 59 (1969).

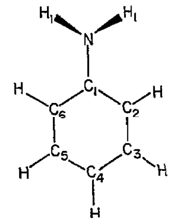
Thiophenol

C_6H_6S C_6H_5SH C_s

Data are consistent with planarity.

[1] K. I. Johansson, H. Oldeberg and H. Selen, Arkiv. Fysik. **33**, 313 (1967).

Aniline



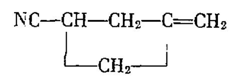
C_6H_7N C_s

Bond	Substitution	Angle	Substitution
NH_1	1.001 D	H_1NH_1	113.1 D
C_1N	1.402 B	$C_6C_1C_2$	119.4 A
C_1C_2	1.397 B	$C_1C_2C_3$	120.1 A
C_2C_3	1.394 B	HC_2C_3	120.1 A
C_3C_4	1.396 B	$C_2C_3C_4$	120.7 A
C_2H	1.082 B	HC_3C_2	119.4 A
C_3H	1.083 B	$C_3C_4C_5$	118.9 A
C_4H	1.080 B		

The C_6H_5N fragment is essentially planar. The dihedral angle between the NH_2 and C_6H_5N planes is 37.5°.

[1] D. G. Lister, J. K. Tyler, J. H. Hog, and N. W. Larsen, J. Mol. Struct. **23**, 253 (1974).
[2] D. G. Lister and J. K. Tyler, Chem. Commun. **1966**, 152 (1966).

3-Methylenecyclobutanecarbonitrile

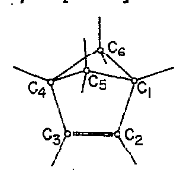


C_6H_7N C_s

The ring is non-planar with the CN group in the equatorial position.

[1] J. R. Durig, Y. S. Li, M. D. Harmony and M. Y. Fong, J. Mol. Struct. **23**, 377 (1974).

Bicyclo[2.1.1]hex-2-ene



C_6H_8 C_{2v}

Bond	Substitution	Angle	Substitution
C_1C_2	1.528 B	$C_1C_2C_3$	103.3 C
C_2C_3	1.341 B	$C_5C_1C_2$	100.4 C
C_1C_5	1.568 B	$C_5C_1C_6$	85.3 C
		$C_1C_5C_4$	81.4 C
		θ^a	126.7 C

[a] Dihedral angle formed by intersection of $C_4C_5C_1$ and $C_4C_6C_1$ planes.

[1] C. S. Wang and M. D. Harmony, J. Am. Chem. Soc. **98**, 1976.

1,3-Cyclohexadiene

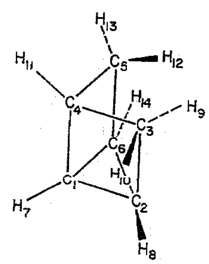
C_6H_8 $H_2C—HC{=}CH—CH{=}CH—CH_2$ C_2

Angle	Effective
τ	17.5 X

τ is the torsional angle between the two double bonds.

[1] S. S. Butcher, J. Chem. Phys. 42, 1830 (1965).

Tricyclo[2.2.0.0^{2,6}]hexane



C_6H_8 C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
C_1C_2	1.513 B	1.518 C	$H_9C_3H_{10}$	110.2 C	110.7 C
C_1C_4	1.584 B	1.589 C	$C_1C_4H_{11}$	126.4 B	126.5 B
C_2C_3	1.523 B	1.527 B	$C_3C_4H_{11}$	120.9 B	120.9 B
C_2C_6	1.533 B	1.541 C	$C_4C_1H_7$	134.6 B	134.5 B
C_3C_4	1.549 B	1.553 B	$C_2C_1H_7$	131.9 B	131.8 B
C_1H_7	1.079 C	1.077 C	$C_1C_2H_8$	127.4 B	127.4 B
C_2H_8	1.082 C	1.080 C	$C_6C_2H_8$	120.6 B	120.5 B
C_3H_9	1.099 C	1.098 C	$C_3C_2H_8$	128.4 B	128.6 B
C_3H_{10}	1.087 C	1.090 C	$C_1C_2C_3$	91.8 B	
C_4H_{11}	1.086 C	1.086 C	$C_2C_3C_4$	86.2 A	
			$C_3C_4C_1$	88.2 A	
			$C_4C_1C_2$	85.4 A	
			$C_1C_2C_6$	59.6 A	
			$C_2C_1C_6$	60.9 A	

[1] R. D. Suenram, J. Amer. Chem. Soc. 97, 4869 (1975).

1-Chloro-3,3-dimethyl-1-butyne (Tertiary Butyl Chloroacetylene)

C_6H_9Cl $(CH_3)_3C^1C^2{\equiv}C^3Cl$ C_{3v}

Bond	Substitution	Effective
C^3Cl	1.638 B	
$C^1\cdots C^3$	2.671 B	
C^1C^2 [a]	1.47 X	1.47 D

[a] $r(C^1C^2)$ calculated assuming $r(C^2C^3)$ is 1.205 Å.

[1] H. Bodenseh, R. Gegenheimer, J. Mennicke and W. Zeil, Z. Naturforsch. 22A, 523 (1967).

Cyclohexene

C_6H_{10} C_2

Stark effect data and rotational constants are consistent with "half-chair" form (C_2 symmetry) for the molecule. Data are insufficient for structure determination.

[1] L. H. Scharpen, J. E. Wollrab, and D. P. Ames, J. Chem. Phys. 49, 2368 (1968).

3,3-Dimethyl-1-butyne (t-Butyl Acetylene)

C_6H_{10} $(C^{(4)}H_3)_3C^{(3)}—C^{(2)}{\equiv}C^{(1)}H$ C_{3v}

Bond	Substitution	Angle	Substitution
$C^{(1)}H$	1.056 A	$C^{(2)}C^{(3)}C^{(4)}$	108.0 C
$C^{(1)}C^{(2)}$	1.209 A		
$C^{(2)}C^{(3)}$	1.496 D		
$C^{(3)}C^{(4)}$	1.532 C		

[1] L. J. Nugent, D. E. Mann and D. R. Lide, Jr., J. Chem. Phys. 36, 965 (1962).

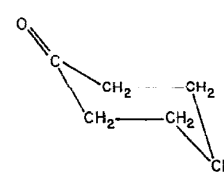
1,1-Difluorocyclohexane

$C_6H_{10}F_2$ C_s

The microwave data show that the molecule adopts the chair conformation.

[1] D. Damiani and L. Ferretti, Chem. Phys. Lett. 24, 357 (1974).

Cyclohexanone

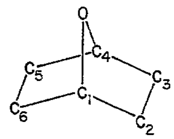


$C_6H_{10}O$ C_s

Rotational constants of assigned transitions are for the "chair" form.

[1] Y. Ohnishi and K. Kozima, Bull. Chem. Soc. Japan 41, 1323 (1968).

7-Oxabicyclo[2.2.1]heptane



$C_6H_{10}O$ C_{2v}

Bond	Substitution	Effective	Angle	Substitution
C_1C_2	1.537 B		$C_1C_2C_3$	101.2 B
C_2C_3	1.551 B		$C_2C_1C_6$	109.9 B
C_1O		1.452 C		

Hydrogen parameters were assumed to obtain the CO distance.

[1] R. A. Creswell, J. Mol. Spectrosc. 56, 133 (1975).

Fluorocyclohexane

$C_6H_{11}F$ C_s

Insufficient data available for structure determination. Both axial and equatorial conformers observed. Ground vibrational state of equatorial form is more stable by 259 ± 28 cal/mol.

[1] L. H. Scharpen, J. Amer. Chem. Soc. **94**, 3737 (1972).

Cyclohexane

C_6H_{12} $CH_2CH_2CH_2CH_2CH_2CH_2$ D_{3d}

Bond	Effective	Angle	Effective
CC	1.535 X	HCH	110.0 X

Conformation is the chair form.

[1] R. A. Peters, W. J. Walker and A. Weber, J. Raman Spectrosc. **1**, 159 (1973).

Hexafluorobenzene

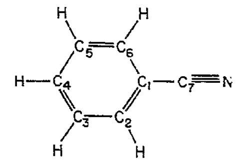
C_6F_6 D_{6h}

Bond	Effective
CF	1.321 X

In order to obtain the CF bond distance it was necessary to assume the CC distance.

[1] J. Schlupf and A. Weber, J. Raman. Spectrosc. **1**, 3 (1973).

Benzonitrile



C_7H_5N C_{2v}

Bond	Substitution	Angle	Substitution
C_1C_2	1.388 C	$C_6C_1C_2$	121.8 C
C_2C_3	1.396 C	$C_1C_2C_3$	119.0 B
C_3C_4	1.397 B	$C_2C_3C_4$	120.1 A
C_1C_7	1.451 B	$C_3C_4C_5$	120.1 A
C_7N	1.158 A	C_3C_2H	120.4 C
C_2H	1.080 C	C_2C_3H	120.0 A
C_3H	1.082 B		
C_4H	1.080 A		

[1] J. Casado, L. Nygaard, and G. O. Sørensen, J. Mol. Struct. **8**, 211 (1971).
[2] B. Bak, D. Christensen, W. B. Dixon, L. Hansen-Nygaard, and J. Rastrup-Andersen, J. Chem. Phys. **37**, 2027 (1962).

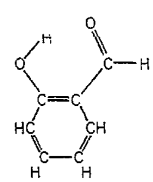
Isocyanatobenzene (Phenylisocyanate)

C_7H_5NO C_6H_5NCO C_s

The microwave data indicate a planar structure with a non-linear C—N=C=O moiety.

[1] A. Bouchy and G. Roussy, C. R. Acad. Sci. Paris **277**, 143 (1973).

Salicylaldehyde

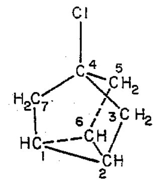


$C_7H_6O_2$ C_s

Bond	Substitution
O ⋯ H	1.76 C

[1] H. Jones and R. F. Curl, Jr., J. Mol. Spectrosc. **42**, 65 (1972).

4-Chloro-tricyclo[2.2.1.0^{2,6}]heptane (4-Chloronortricyclene)



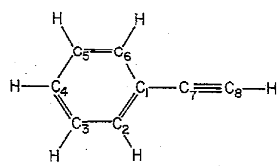
C_7H_9Cl C_{3v}

Bond	Substitution	Angle	Substitution
C_4Cl	1.763[a]	ClC_4C_7	115.7 D
C_7C_4	1.538 D	$C_7C_4C_3$	102.6 B
C_1C_7	1.525 D	$C_1C_7C_4$	96.2 C
C_1C_2	1.527 B	$C_2C_1C_7$	106.6 C

[a] This distance was assumed with an uncertainty of ±0.003 Å in order to determine the C_4 substitution coordinate.

[1] V. W. Laurie and W. M. Stigliani, J. Am. Chem. Soc. 95, 4154 (1973).

Ethynyl benzene (Phenyl acetylene)



C_8H_6 C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
C_1C_2		1.388 C	$C_2C_1C_6$		120.8 C
C_2C_3		1.396 D	$C_1C_2C_3$		119.8 B
C_3C_4	1.398 A		$C_2C_3C_4$		119.9 B
C_1C_7		1.448 C	$C_3C_4C_5$	119.9 A	
C_7C_8	1.208 A				
C_8H	1.055 A				

Ring CH parameters were assumed for calculation of effective bond distances and angles.

[1] A. P. Cox, I. C. Ewart, and W. M. Stigliani, J. Chem. Soc. Faraday Trans. II. 71, 504 (1975).

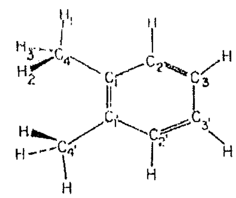
7-Methylene-1,3,5-cycloheptatriene (Heptafulvene)

C_8H_8 C_{2v}

The observed microwave spectrum confirmed the planar conformation.

[1] A. Bauder, C. Keller and M. Neuenschwander, J. Mol. Spectrosc. 63, 281 (1976).

ortho-Xylene



C_8H_{10} C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
C_4H_1	1.080 B		$H_1C_4H_2$	108.9 C	
C_4H_2	1.095 B		$H_2C_4H_3$	106.0 D	
C_1C_4		1.509 X	$C_4C_1C_{1'}$		121.1 X
C_1C_2		1.414 X	$C_2C_1C_{1'}$		119.8 X
$C_1C_{1'}$		1.394 X	C_1C_2H		118.9 X
C_2H		1.072 X	C_2C_3H		119.7 X
C_3H		1.079 X	$H_1C_4C_1$		111.2 X
			$H_2C_4C_1$		111.0 X

[1] H. D. Rudolph, K. Walzer and I. Krutzik, J. Mol. Spectrosc. 47, 314 (1973).

1-Cyanoadamantane

$C_{11}H_{15}N$ $C_{10}H_{15}CN$ C_{3v}

Bond	Substitution	Effective	Angle	Effective
CN	1.159 A		CCC	109.5[a]
CC		1.543 X	HCH	109.5[a]
CC(N)		1.466 X		
CH		1.09[a]		

All CC bonds were assumed to be equal.

[a] Assumed values.

[1] D. Chadwick, A. C. Legon and D. J. Millen, J. Chem. Soc. Faraday Trans. 68, 2064 (1972).