

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_o) 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.

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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 resonance 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.

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The critical task of supplying the necessary bibliographic support has been performed by the National Bureau of Standards, although the Lndolt-Börnstein tables [1, 2] 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_0 , 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:

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

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 ;

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

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:

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

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 k th vibrational mode, respectively; v stands for $v_1, v_2, \dots, v_{3N-6}$. In eq (3) A_c is the A rotational constant for the hypothetical equilibrium configuration of the molecule; that is,

$$A_c = h/8\pi^2 I_a^{(c)} \quad (4)$$

where $I_a^{(c)}$ 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_c, C_v , and C_c . For any vibrational state v ,

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

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 \mathbf{P} with components defined as follows:

$$P_{\alpha\beta} = \sum_{i=1}^N m_i \alpha_i \beta_i \quad (6)$$

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 \mathbf{P} and are related to the principal moments of inertia, as follows:

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

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

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

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—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_o structure. For example, Costain [12] has shown that $r_s \approx \frac{1}{2}(r_o + r_e)$ for diatomic molecules.

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

$$I_\eta^{(m)} = 2I_\eta^{(s)} - I_\eta^{(o)} \quad (14)$$

in which $I_\eta^{(s)}$ 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 $I^{(a)}$ for the average configuration can be derived from $I^{(o)}$ values. The bond distances and bond angles derived from the $I^{(a)}$ 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 $I^{(a)}$ moments for a single isotopic species and those determined from $I^{(a)}$ 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_o (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_θ	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_θ parameters—the true ground vibrational state average values of distances and angles. The r_θ 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_θ 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_o 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_o 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_o 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

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

and

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

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

$$\Delta_{aa} = 2(P_{aa}^{(e)} - P_{aa}^{(o)}) \quad (17)$$

from which it follows that, upon isotopic substitution,

$$\begin{aligned} \Delta P_{aa}^{(o)} &= P_{aa}^{(o)'} - P_{aa}^{(o)} \\ &= P_{aa}^{(e)'} - P_{aa}^{(e)} - (\Delta'_{aa} - \Delta_{aa})/2. \end{aligned} \quad (18)$$

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

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

If the value $0.006 \text{ u} \cdot \text{\AA}^2$ is used for the difference in the pseudoinertia defect upon isotopic substitution, it is found that

$$\delta a_s/\text{\AA} = \pm \left| \frac{0.0015}{a_s' \text{\AA}} \right|. \quad (20)$$

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_o parameters.

The choice of $0.006 \text{ u} \cdot \text{\AA}^2$ for $\delta\Delta P_{aa}$ 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_{aa} is an appreciable fraction of $0.006 \text{ u} \cdot \text{\AA}^2$ 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_o 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 i th, and j th nuclei this leads to an uncertainty

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

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_o 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:

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

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_o 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	$\leq \pm 0.002$	$\leq \pm 0.2$
B	$\pm 0.002 - \pm 0.005$	$\pm 0.2 - \pm 0.5$
C	$\pm 0.005 - \pm 0.010$	$\pm 0.5 - \pm 1.0$
D	$\pm 0.010 - \pm 0.020$	$\pm 1.0 - \pm 2.0$
E	$\pm 0.020 - \pm 0.050$	$\pm 2.0 - \pm 5.0$
X	unable to evaluate, unknown, or un- reliable	

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 $I_0^{(2)}$ from $I_0^{(0)}$. 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 C₁, C₂, C₃, 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_o), or average (r_z), and are separated into distance and angle categories. As a general rule, r_s , r_e , and r_z parameters are always listed when available; r_o 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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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	II _n	2.756	2.754
AlI	2.540	2.537	CLi	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*	ClTi	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	FI _n	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	FTI	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*	Gal	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, ²HLi.

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·H ₂		Undefined
Bond	Effective	Angle	Effective	

Mean distance between center of mass of H₂ 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 ²B₁.

[1] R. N. Dixon, G. Duxbury and H. M. Lambertson, *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 BF	1.728 C	1.315 C	FBF	118.1 C	

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

Difluoroborane

BF ₂ H			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 ₂ HO		F ₂ BOH		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	

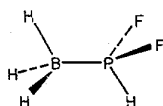
[1] H. Takeo and R. F. Curl, *J. Chem. Phys.* **56**, 4314 (1972).

1,1-Difluoroboranimine (Aminodifluoroborane)

BF ₂ H ₂ N			BF ₂ NH 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 ₂ H ₂ P			C _s			
Bond	Substitution	Effective	Angle	Substitution	Effective	
PH		1.409 C	H _a BH _a	112.7 C		
PF		1.552 C	H _a BH _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 ₂ O		F ₂ BO		C _{2v}	
Bond	Effective	Angle	Effective		
BF	1.30 E	FBF	126 E		
BO	1.40 E				

Ground electronic state is ³B₂.

[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 ₂ H ₃ P		F ₃ B-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 ₃ H ₃ P			F ₃ PBH ₃			C _{3v}	
Bond	Substitution	Effective	Angle	Substitution	Effective		
BH	1.207 B		HBH	115.1 C			
PF		1.538 D	FPH		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 _{2v}
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 ²B₁.

[1] G. Herzberg and J. W. C. Johns, *Proc. Roy. Soc. (London)* **A298**, 142 (1967).

Phosphine-Borane

BH ₂ P		H ₂ BPH ₂		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	

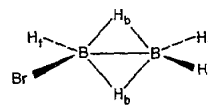
[1] J. R. Durig, Y. S. Li, L. A. Carreira, and J. D. Odom, *J. Amer. Chem. Soc.* **95**, 2491 (1973).

Boron Dioxide

BO ₂		OBO		D _{∞h}
Bond		Effective		
BO		1.265 A		

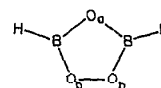
Ground electronic state is ²Π_g.

[1] I. W. C. Johns, *Can. J. Phys.* **39**, 1738 (1961).

Bromodiborane(6)

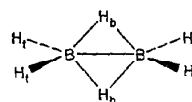
B ₂ BrH ₅				C _{2v}
Bond	Substitution	Effective	Angle	Substitution Effective
BB	1.773 B		BBBr	121.4 C
BBr	1.930 B		BBH ₁	119.9 X
H ₁ H ₂		1.954 X	H ₂ BH ₂	95.6 X
BH ₁		1.196 X	BH ₂ B	84.4 X

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

1,2,4,3,5-Trioxadiborolane

B ₂ H ₂ O 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 _b O _b	1.470 A	HBO _a	126.3 C	

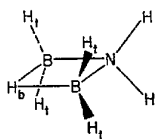
[1] W. V. F. Brooks, C. C. Costain and R. F. Porter, *J. Chem. Phys.* **47**, 4186 (1967).

Diborane(6)

B ₂ H ₆				D _{2h}
Bond	Effective	Angle	Effective	
B...B	1.763 C	H ₁ BH ₁	121.0 C	
B-H ₁	1.201 C	H ₂ BH ₂	96.2 C	
B-H ₂	1.320 C			

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

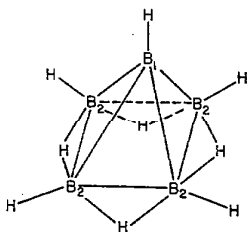
Aminodiborane



B ₂ H ₇ N						C _{2v}	
Bond	Substitution	Effective	Angle	Substitution	Effective		
DB	1.916 B		BNB	75.9 A			
BN	1.558 B		BH ₃ B	90.0 B			
BH _b	1.355 C		H _i BH _i	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)



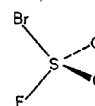
B ₅ H ₉		C _{4v}	
Bond		Effective	
B ₁ B ₂		1.687 C	
B ₂ B ₂		1.800 C	

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).

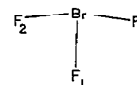
Sulfuryl bromide fluoride



BrFO ₂ S				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 ₁ BrF ₂	86.2 C		
BrF ₂	1.810 B				

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

Bromotrifluorosilane

BrF ₃ Si		SiF ₃ Br		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 ₅ S		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		BrCeH 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 ₂ Si		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 ₂ Sn		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 ₃ FSi		FSiBr ₃		C _{3v}	
Bond	Effective	Angle	Effective		
SiBr	2.171 X	BrSiBr	111.6 X		

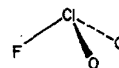
SiF = 1.560 was assumed.

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

Tribromosilane

Br ₃ HSi		Br ₂ SiH		C _{3v}	
Bond	Effective	Angle	Effective		
SiH	1.494 C	BrSiBr	111.6 E		
SiBr	2.170 E				

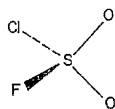
[1] M. Mitzlaff, R. Holm, and H. Hartmann, *Z. Naturforsch.* **23a**, 65 (1968).

Chloryl fluoride

ClFO ₂		C _s	
Bond	Substitution	Angle	Substitution
ClF	1.696 B	OCIO	115.2 A
ClO	1.418 B	FCIO	101.7 A

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

Sulfuryl chloride fluoride

ClFO₂S C_s

Bond	Effective	Angle	Effective
SO	1.408 ^a	OSO	123.7 X
SF	1.550 X	FSCI	99.0 ^a
SCI	1.985 X	OSF	107.5 X
		OSCI	107.5 X

^a Assumed values.

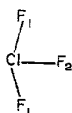
[1] C. S. Holt and M. C. L. Gerry, Chem. Phys. Lett. 9, 621 (1971).

Phosphorous chloride difluoride
(Chlorodifluorophosphine)ClF₂P PF₂Cl C_s

Bond	Effective	Angle	Effective
PF	1.571 B	FPF	97.3 B
PCI	2.030 C	FPCI	99.2 C

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

Chlorine Fluoride

ClF₃ C_{2v}

Bond	Effective	Angle	Effective
ClF ₁	1.598 B	F ₁ ClF ₂	87.5 B
ClF ₂	1.698 B		

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

Chlorotrifluorogermane

ClF₂Ge GeF₂Cl 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

ClF₂Si SiF₂Cl 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

ClF₅ C_{4v}

Bond	Effective	Angle	Effective
ClF	1.65 X	F _{ax} ClF _{eq}	86.5 X
		F _{eq} ClF _{eq}	89.9 X

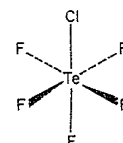
The ClF_{ax} and ClF_{eq} distances have been assumed to be equal.

[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

ClF₅Te 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_{ax} distance.

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

Tungsten pentafluoride chloride

ClF ₂ W		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 ₂ N		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 ₃ Si			H ₃ SiCl			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 ₃ Sn		H ₃ SnCl		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).

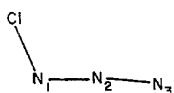
Thiazyl chloride

CINS			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			
SCI	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 ₁ N ₂	108.7 C		
N ₁ N ₂	1.252 C	N ₁ N ₂ N ₃	171.9 C		
N ₂ N ₃	1.133 C				

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

Chlorine dioxide

ClO ₂			ClOClO			C _{2v}		
Bond	Substitution	Average	Angle	Substitution	Average			
ClO	1.471 B	1.476 B	ClOClO	117.6 B	117.5 B			

Ground state is ²B₁.

[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. C. 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 ₃ Re		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 ₂ H ₂ Si		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 ₂ O			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 ₂ S				C _{2v}			
Bond	Substitution	Average	Effective				
ClS	2.014 A	2.015 A	2.014 A				

Angle	Substitution	Average	Effective				
ClSCl	102.6 A	102.7 A	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 ₂ FSi		FSiCl ₂		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. Naturforsch.* **22a**, 1287 (1967).

Trichlorogermane

Cl ₃ GeH		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 ₃ HSi			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	2.019 A	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. Naturforsch.* **22a**, 1415 (1967).

Nitrogen trichloride

Cl ₃ N			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 ₃ OP			C _{3v}		
Bond	Effective	Angle	Substitution		
PO	1.455 D	ClPCI	103.7 C		
PCI	1.989 C				

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

Vanadyl(V) chloride

Cl ₃ OV		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 ₃ P		PCl ₃		C _{3v}	
Bond	Effective	Angle	Effective		
PCI	2.043 B	ClPCI	100.1 C		

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

Cesium Hydroxide

CsHO		CsOH		C _{∞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. Kuczowski, *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 ₃ Si		SiH ₃ F		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 ₂ Si ₂		H ₂ Si-SiH ₂ F			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 SiH₂F' 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 ₃ Re		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 ₂ Ge		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 ₂ HN				C _s
Bond	Effective	Angle	Effective	
NF	1.400 B	FNF	102.9 B	
NH	1.026 B	HNF	99.8 B	

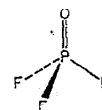
[1] D. R. Lide, Jr., *J. Chem. Phys.* **38**, 456 (1963).
 [2] S. Sundaram, *Proc. Phys. Soc.* **92**, 261 (1967).

Difluorophosphine

F ₂ HP				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 ₂ HPO				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).

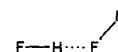
Hydrothiophosphoryl difluoride



F ₂ HPS				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

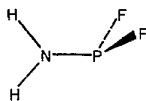


F₂H₂ C_s

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).

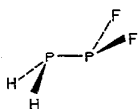
Phosphoramidous difluoride
(Aminodifluorophosphine)



F ₂ H ₂ NP			
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 ₂ H ₂ P 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 ₂ Kr		KrF ₂		D _{∞h}
Bond	Effective			
KrF	1.875 D			

Two possible *J* assignments of the ν_3 band of KrF₂ 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).

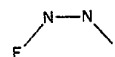
Difluoroamidogen
(Nitrogen difluoride)

F ₂ N					
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 ²B₁.

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

cis-Difluorodiazine



F ₂ N 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 ₂ O			
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 ₂ OS			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 ₂ OSe			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 ₂ O 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 ₂ O ₂ S		F ₂ SO 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. Friston, J. Chem. Phys. **26**, 734 (1957).

Sulfur Difluoride

F ₂ S			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 ₂ SO			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 ₂ S 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 ₂ S ₂			S-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 ₂ Si			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 ₂ Xe		D _{oh}	
Bond	Effective	Angle	Effective
Xe-F	1.977 B		

[1] S. Reichman and F. Schreiner, *J. Chem. Phys.* **51**, 2855 (1969).

Trifluorosilane

F ₃ HSi			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 ₃ H ₂ Si ₂			F ₃ Si-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 ₃ ISi		F ₃ SiI		C _{3v}	
Bond	Effective	Angle	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**, 1814 (1967).

Nitrogen Trifluoride

F ₂ N			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 ₂ NS		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 ₃ OP		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 ₃ P				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	

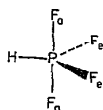
- [1] Y. Kawashima and A. I. Cox, *J. Mol. Spectrosc.* **65**, 319 (1977).
 [2] E. Hirota and Y. Morino, *J. Mol. Spectrosc.* **33**, 460 (1970).

Thiophosphoryl Fluoride

F ₃ PS				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 ₄ HP				C _{2v}
Bond	Effective	Angle	Effective	
PF _a	1.596 B	HPF _a	90 E	
PF _e	1.55 E	HPP _e	124 D	

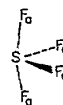
- The PH distance was assumed.
 [1] S. B. Pierce and C. D. Cornwell, *J. Chem. Phys.* **48**, 2118 (1968).

Xenon Tetrafluoride Oxide

F ₄ OXe		OXeF ₄		C _{4v}
Bond	Substitution	Effective	Angle	Effective
XeO	1.703 D	1.900 B	OXeF	91.8 C
XeF				

- [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).

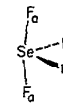
Sulfur Tetrafluoride



F ₄ S				C _{2v}
Bond	Effective	Angle	Effective	
SF _a	1.646 B	F _a SF _e	101.5 C	
SF _e	1.545 B	F _e SF _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 ₄ Se				C _{2v}
Bond	Effective	Angle	Effective	
SeF _a	1.771 C	F _a SeF _e	100.5 C	
SeF _e	1.682 C	F _e SeF _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).

Iodogermene

GeH ₃ I		IGeH ₃		C _{3v}
Bond	Effective		Effective	
GeI	2.508 B			

- H₂Ge projection on C₃ axis was assumed.
 [1] S. N. Wolf and L. C. Krisher, *J. Chem. Phys.* **56**, 1040 (1972).

Germane

GeH₄ 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

GeH₃Si H₃GeSiH₃ C_{3v}

Bond	Effective
GeSi	2.357 X

Parameters for the GeH₃ and SiH₃ groups were assumed.
[1] A. P. Cox and R. Varma, J. Chem. Phys. 46, 1603 (1967).

Iodosilylene

HHSi 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).

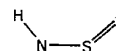
Nitrosyl Hydride

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).

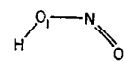
cis-Thionylimide

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).

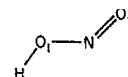
cis-Nitrous Acid

HNO₂ C_s

Bond	Effective	Angle	Effective
HO ₁	0.982 D	O ₁ NO ₂	113.6 D
NO ₁	1.392 D	HO ₁ N	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

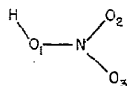
HNO₂ C_s

Bond	Substitution	Angle	Substitution
H-O ₁	0.958 C	O ₁ NO ₂	110.7 C
N-O ₁	1.432 C	HO ₁ N	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. Kuczowski, J. Amer. Chem. Soc. 88, 5071 (1966).

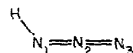
Nitric Acid



HNO ₃		C _s	
Bond	Substitution	Angle	Substitution
HO ₁	0.964 C	HO ₁ N	102.2 C
NO ₁	1.406 C	O ₁ NO ₂	115.9 C
NO ₂	1.211 C	O ₁ NO ₃	113.8 C
NO ₃	1.199 C	O ₂ NO 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 ₁ H	0.975 X	HN ₁ N ₂	114.1 X
N ₁ N ₂	1.237 X		
N ₂ N ₃	1.133 X		

The N₃ 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 (1969).
 [2] C. Matsumura and D. R. Lide, Jr., *J. Chem. Phys.* **50**, 30 (1969).

Hydroperoxyl radical

HO ₂		Angle	Effective
Bond	Effective		
HO	0.977 C	HOO	104.1 D
OO	1.335 C		

Ground state is ²A₁.

- [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. Howard, *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 ₂ Kr		Undefined
Bond	Effective	
Mean value between center of mass of H ₂ and Kr atom	4.07 X	

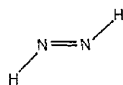
- [1] A. R. W. McKellar and H. L. Welsch, *J. Chem. Phys.* **55**, 595 (1971).

Amidogen

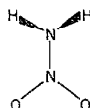
H ₂ N		C _{2v}	
Bond	Effective	Angle	Effective
NH	1.024 C	HNH	103.3 B

Ground electronic state is ²B₁.

- [1] K. Dressler and D. A. Ramsay, *Phil. Trans. Roy. Soc. (London)* **A251**, 553 (1959).

trans-Diazine (Diimide)H₂N₂ C_{2h}

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

[1] M. Carloti, J. W. C. Johns and A. Trombetti, *Can. J. Phys.* **52**, 340 (1974).**Nitramide**H₂N₂O₂ C_s

Bond	Effective	Angle	Effective
NN	1.427 X	HNH	115.2 X
NH	1.005 X	ONO	130.1 X
		∠ ^a	51.8 X

^a Angle between NH₂ and NNO₂ planes.[1] J. K. Tyler, *J. Mol. Spectrosc.* **11**, 39 (1963).**Hydrogen Neon(1/1)**H₂Ne 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**H₂O 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**H₂O⁺ C_{2v}

Bond	Effective	Angle	Effective
OH	0.999 C	HOH	110.5 B

Ground electronic state is ²B₁.[1] H. Lew and I. Heiber, *J. Chem. Phys.* **58**, 1246 (1973).**Hydrogen Peroxide**H₂O₂ C₂

Angle	Effective ^a
Dihedral	120 X

^a Average dihedral angle in the lowest (N = 0, τ = 1, 2) internal rotation states.[1] W. C. Oelfke and W. Gordy, *J. Chem. Phys.* **51**, 5336 (1969).**Phosphino**H₂P C_{2v}

Bond	Effective	Angle	Effective
PH	1.418 C	HPH	91.7 B

Ground electronic state is ²B₁.[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 ₂ S				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 ₂ S ⁺				C _{2v}	
Bond	Effective	Angle	Effective		
SH	1.358 C	HSH	92.9 B		

Ground electronic state is ²B₁.

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

Hydrogen Disulfide (Disulfane)

H ₂ S 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 ₂ Se			
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 constants of Ref. 1. The error is based on the spread in the dimensions calculated from the I_A, I_B, I_C ; or I_A, I_C pairs. The average structure 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 obtained from the various pairs of parameters. Lines from Ref. 3 were included with infrared data in Ref. 1 to obtain the rotational constants.

[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 ₂ Si				C ₂	
Bond	Effective	Angle	Effective		
SiH	1.516 C	HSiH	92.1 B		

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

Hydrogen Telluride

H ₂ Te						C _{2v}	
Bond	Effective	Equilibrium	Angle	Effective	Equilibrium		
HTe	1.653 D	1.658 B	HTeH	90.3 D	90.2 B		

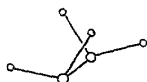
[1] N. K. Moncur, P. D. Willson, and T. H. Edwards, *J. Mol. Spectrosc.* **52**, 380 (1974).

Stibine

H ₃ Sb			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

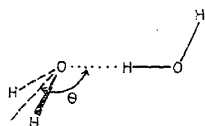
H ₄ N ₂				C ₂			
Bond	Effective	Angle	Effective				
NH	1.008 D	HNH	113.3 D				
NN	1.447 B	HNN	109.2 D				
		ϕ^a	88.9 D				

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 ₂ O ₂		C _s	
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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 ₄ P ₂		H ¹ H ² P-PH ² H ¹		C ₂	
Bond	Effective	Angle	Effective		
PP	2.219 B	H ₁ PH ₂	92.0 C		
PH ₁	1.414 C	H ₁ PP	94.3 B		
PH ₂	1.417 C	H ₂ PP	99.1 B		
		ϕ^a	74.0 E		

^a Dihedral angle measured from *cis* position. Hydrogens numbered H₂ 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 ₄ Si			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 ₄ Sn		T _d	
Bond	Effective		
SnH	1.711 B		

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

Disilane

H ₆ Si ₂		H ₃ SiSiH 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 ²A₁.
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 ₂ O		N—N—O		C _{∞v}	
Bond		Equilibrium			
NN		1.128 A			
NO		1.184 A			

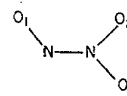
- [1] K. Narahari Rao, *Ann. New York Acad. Sci.* **220**, 17 (1973).
[2] C. A. Burrus and W. Gordy, *Phys. Rev.* **101**, 599 (1956).
[3] C. H. Townes and A. L. Schawlow, *Microwave Spectroscopy*, McGraw-Hill, New York (1955).

Dinitrogen Oxide(+1) Ion

N ₂ O ⁺		NNO ⁺		C _{∞v}	
Bond		Effective			
NN		1.155 C			
NO		1.185 C			

Ground electronic state is ²Π₁.
[1] J. H. Callomon and F. Creutzberg, *Phil. Trans. Roy. Soc.* **A277**, 157 (1974).

Dinitrogen trioxide



N ₂ O 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. Kuczowski, *Trans. Faraday Soc.* **65**, 1963 (1969).

Azido

N ₃		D _{∞h}	
Bond		Effective	
NN		1.181 A	

Ground electronic state is ²Π_g.
[1] A. E. Douglas and W. J. Jones, *Can. J. Phys.* **43**, 2216 (1965).

Disulfur monoxide

OS ₂			S ₂ O			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 ₂ S		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. Steenbeekeliers, *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 ₂ S 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 ₂ Se		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).

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Sulfur Trioxide

O ₃ S		D _{3h}	
Bond	Effective		
SO	1.420 A		

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

C₁ Molecules

Cyanogen bromide

CBrN		BrCN		C _{∞v}	
Bond	Substitution	Equilibrium			
B ₁ C	1.769 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 ₂ O		C _{2v}			
Bond	Effective	Angle	Effective		
CO	1.172 C	BrCBr	112.3 C		
CBr	1.917 C				

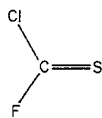
- [1] J. H. Carpenter, J. G. Smith, J. Thompson and D. H. Whiffen, *J. C. S. Faraday Trans.* **1976**, 384 (1976).

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).

Chlorofluorothiocabonyl

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
CICS	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

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

CCINO		CINCO		C _s
Bond	Substitution	Angle	Substitution	
CIN	1.705 B	CINC	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 ₂ F ₂			Cl ₂ CF ₂			C _{2v}
Bond	Substitution	Effective	Angle	Substitution	Effective	
CCl	1.744 C		CICCl	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 ₂ O		COCl ₂		C _{2v}
Bond	Effective	Angle	Effective	
CO	1.166 B	CICCl	111.3 B	
CCl	1.746 B			

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

Trichlorofluoromethane

CCl ₃ F		C _{3v}	
Bond	Effective	Angle	Effective
CCl	1.76 C	CICCl	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_{2v}
Bond	Substitution	Effective	
CF		1.262 B	
CN	1.159 B		

[1] J. K. Tyler and J. Sheridan, *Trans. Faraday Soc.* **59**, 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 ₂ N		F ₂ CN	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 ₂ NP		PF ₂ CN	C_s
Bond	Substitution	Effective	Angle
PF	1.566 C	1.567 C	FPF
PC	1.815 B	1.811 B	FPC
CN	1.157 B	1.158 B	PCN
			Effective
			99.2 B
			99.1 B
			96.9 B
			97.1 B
			171.2 D
			171.5 C

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

Difluorocyanamide

CF ₂ N ₂		NF ₂ CN		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 NF₂ moiety.

^b A mixed r_{01} , r_{02} parameter.

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

Carbonic difluoride
(Carbonyl fluoride)

CF ₂ O		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_{01} , r_{02} 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).

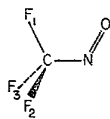
[5] J. H. Carpenter, *J. Mol. Spectrosc.* **50**, 182 (1974).

Carbonothioic Difluoride
(Thiocarbonyl Fluoride)

CF ₂ S		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

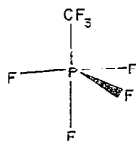
CF₃NOC_s

Bond	Effective	Angle	Effective
CF	1.324 C	F ₁ CN	113.9 D
NO	1.198 C	F ₂ CN	107.5 C
CN	1.512 D	F ₂ CF ₃	109.8 C
		CNO	112.4 C

CF bond distances assumed equal. CF₃ 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

CF₃PC_{3v}

CF₃ shown to be axially substituted.

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

Tribromomethane

CHBr₃HCBBr₃C_{3v}

Bond	Effective	Angle	Effective
CH	1.068 D	BrCB-	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

CHClF₂C_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

HCICO

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

CHCl₂FC_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 ₂		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 _{∞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 _{∞v}
Bond	Substitution	Effective	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 _{∞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 D	
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 _{∞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 ³B₁.

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

Dibromomethane

CH ₂ Br 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 ₂ ClF		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 ₂ Cl 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 ₂ FN	HCN ... HF	C _{∞v}
--------------------	------------	-----------------

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

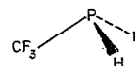
[1] A. C. Legon, D. J. Millen and S. C. Rogers, *Chem. Phys. Lett.* **41**, 137 (1976).

Difluoromethane

CH ₂ F 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**, 354B (1952).

(Trifluoromethyl)phosphine

CH ₂ F ₃ P		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 ₂ N ₂		H ₂ C=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.

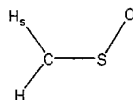
[3] C. B. Moore, *J. Chem. Phys.* **39**, 1884 (1963).

Formaldehyde

CH ₂ O		H ₂ CO		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).

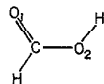
[2] T. Oka, *J. Phys. Soc. Japan* **15**, 2274 (1960).

Methanethial S-oxide
(Sulfine)

CH ₂ OS		C _s	
Bond	Substitution	Angle	Substitution
CH _s	1.085 C	HCH	121.9 C
CH	1.077 C	H _s CS	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 ₂ O 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 ₂ S		H ₂ CS		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 ²A₂'.

The bond length is derived from B₀ of CD₃.

[1] G. Herzberg, *Proc. Roy. Soc. A* **262**, 291 (1961).

Carbon Monoxide-Borane
(Borane carbonyl)

CH ₃ BO		H ₃ BCO		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 ₃ Br		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 ₃ BrHg		H ₃ CH ₂ Br		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).

Chloromethane

CH ₃ Cl			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

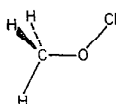
CH ₃ CHg			H ₃ CHgCl		C _{3v}	
Bond	Substitution	Effective	Angle	Effective		
HgC	2.055 D	2.052 C	HCH	109.7 C		
HgCl	2.283 D	2.285 C				
CH		1.092 C				

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

[2] J. T. Cox, T. Gaumann 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 ₃ ClO		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 CH₃ 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).

Methanesulfonyl chloride

CH ₃ ClS		H ₃ CSCl		C _s
Bond	Substitution	Effective	Angle	Effective
SCl	2.030 B	2.037 B	CISC	99.4 B
CS		1.788 B	θ ^a	110.2 X
CH		1.082 C		

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 ₃ Cl ₃ Ge		H ₃ CGeCl ₃		C _{3v}
Bond	Substitution	Angle	Substitution	
GeCl	2.135 C	CCeCl	106.0 C	

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

Methyltrichlorosilane

CH ₃ Cl ₃ Si		H ₃ C-SiCl ₃		C _{3v}
Bond	Effective	Angle	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.

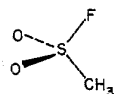
[1] R. C. Mockler, J. H. Bailey and W. Gordy, *J. Chem. Phys.* **21**, 1710 (1953).

[2] M. Mitzlaff, R. Holm and H. Hartmann, *Z. Naturforsch.* **22**, 1415 (1967).

Fluoromethane

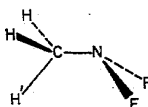
CH ₃ F		C _{3v}	
Bond	Substitution	Angle	Substitution
CF	1.383 A	HCH	110.6 B
CH	1.100 B		

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

Methanesulfonyl FluorideCH₃FO₂SC_s

Except for symmetry no structural results were obtained.

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

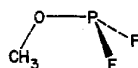
N,N-DifluoromethylamineCH₃F₂NC_s

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.

CH₃ and NF₂ group are staggered.

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

**Phosphorodifluoridous acid methyl ester
(Methoxydifluorophosphine)**CH₃F₂OPC_s

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

* This distance is r_s.

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

Methyldifluorophosphine

CH ₃ F ₂ P		CH ₃ PF 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. Coddling, R. A. Creswell and R. H. Schwendeman, *Inorg. Chem.*, **13**, 856 (1974).

Methyltrifluorosilane

CH ₃ F ₃ Si			H ₃ CSiF 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 ₃ GeN		H ₃ GeCN		C _{3v}
Bond	Substitution	Substitution	Substitution	
GeC		1.919 B		
CN		1.155 B		

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

Iodomethylmercury

CH ₃ HgI			H ₃ CHgI		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			

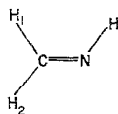
[1] C. Walls, D. G. Lister, and J. Sheridan, *J. Chem. Soc., Faraday Trans.*, **71**, 1091 (1975).

Methyl iodide

CH ₃ I			
Equilibrium		Angle	Equilibrium
Bond			
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.* **33**, 1 (1971).
 [9] E. W. Jones, R. J. L. Popplewell and H. W. Thompson, *Proc. Roy. Soc. A* **288**, 39 (1965).
 [10] J. W. Simmons and J. H. Goldstein, *J. Chem. Phys.* **20**, 122 (1952).

Methyleneimine

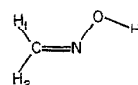


CH ₂ N					
Bond	Substitution		Angle	Substitution	
		Effective			Effective
CN	1.273 C		CNH	110.5 E	
NH	1.023 D		HCH		116.9 C
CH ₁		1.103 D	NCH ₁		123.4 X
CH ₂		1.081 D	NCH ₂		119.7 X

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).

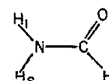
Formaldoxime



CH ₂ NO			
Bond	Substitution	Angle	
			Substitution
C-N	1.276 B	H ₁ CN	121.8 C
NO	1.408 B	H ₂ CN	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 ₂ NO			
Bond	Substitution	Angle	
			Substitution
CN	1.352 D	H ₁ NH ₂	121.6 C
CO	1.219 D	H ₁ NC	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 -NH₂ and -ND₂ 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).

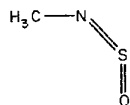
Nitrosomethane

CH ₃ NO		H ₃ C-N-O	C _s
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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

CH₃NOS 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).

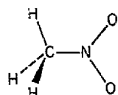
Isocyanatosilane

CH₃NOSi H₃SiN=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

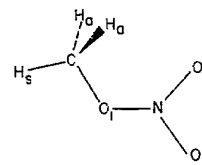
CH₃NO₂ C_s

Bond	Substitution	Angle	Substitution
CN	1.439 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).

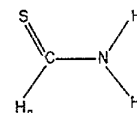
Methyl Nitrate

CH₃NO₃ C_s

Bond	Substitution	Angle	Substitution
CH _a	1.095 C	H _a CH _a	109.8 C
CH _b	1.088 C	H _b CO	103.4 C
CO	1.437 B	H _a CO	110.4 C
NO ₁	1.402 B	CON	112.72 B
NO ₂	1.205 B	O ₁ NO ₂	118.10 B
NO ₃	1.208 B	O ₂ NO ₃	129.52 B

Heavy atoms are coplanar. Methyl group is tilted away from O₂ by 4.8 ± 1°. Axis of NO₂ group is also tilted away from CH₃ 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

CH₂NS C_s

Bond	Substitution	Angle	Substitution
NH _c	1.002 C	H _c NH _t	120 D
NH _t	0.99 D	H _c NC	117.9 B
CN	1.358 B	H _t NC	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 ₃ NSSi		H ₃ SiNCS		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).

Silane carbonitrile

CH ₃ NSi		SiH ₃ CN		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).

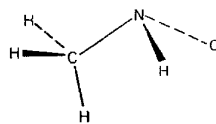
Methane

CH ₄			T _d
Bond	Effective	Substitution	
CH	1.094 A	1.092 A	

The r_e 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 CH₃D.

[1] G. Tarrago, M. Dang-Nhu and G. Poussigues, *J. Mol. Spectrosc.* **49**, 322 (1974).

[2] W. B. Olson, *J. Mol. Spectrosc.* **43**, 190 (1972).

N-Chloromethylamine

CH ₃ CIN		C _i	
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 ₃ Cl ₂ Si		CH ₃ SiHCl 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	CiSiCl	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).

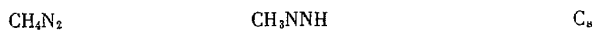
Methyldifluorosilane

CH ₃ F ₂ Si		CH ₃ SiF ₂ H		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 CH₃ group assumed.

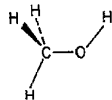
[1] L. C. Krisher and L. Pierce, *J. Chem. Phys.* **32**, 1619 (1960).

[2] J. D. Swalen and B. P. Stoicheff, *J. Chem. Phys.* **28**, 671 (1958).

trans-Methyldiimide

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

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

Methanol

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 CH₃ 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).

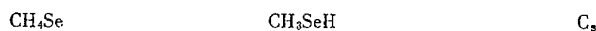
[3] Y. Y. Kwan and D. M. Dennison, *J. Mol. Spectrosc.* **43**, 291 (1972).

Methanethiol

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.

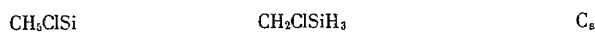
[1] T. Kojima, *J. Phys. Soc. Japan* **15**, 1284 (1960).

Methaneselenol

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 $1.5 \pm 1.0^\circ$. See methanol for definition.

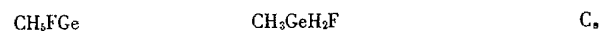
[1] C. H. Thomas, *J. Chem. Phys.* **59**, 70 (1974).

Chloromethylsilane

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.

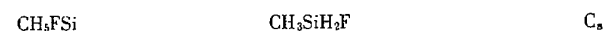
[1] R. H. Schwendeman and G. D. Jacobs, *J. Chem. Phys.* **36**, 1251 (1962).

Methylmonofluorogermane

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		

$\text{GeH} = 1.525 \text{ \AA}$, $\text{HGeH} = 110^\circ$, and $\text{CGeH} = 108.9^\circ$ were assumed in order to determine GeF and FGeC. The CH₃ group was assumed to be symmetrical. There is evidence from the internal rotation that the CH₃ group is tilted 1.9° toward the F atom.

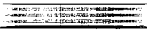
[1] R. F. Roberts, R. Varma, and J. F. Nelson, *J. Chem. Phys.* **64**, 5035 (1976).

Methylfluorosilane

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 CH₃ group was assumed.

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



Methylsilane

CH ₃ Si		CH ₃ SiH 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			

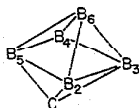
[1] R. W. Kilb and L. Pierce, *J. Chem. Phys.* **27**, 108 (1957).

Methylstannane

CH ₃ Sn		CH ₃ SnH 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



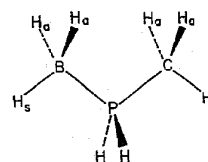
CH ₇ B ₅		C ₆	
Bond	Substitution		
B ₂ B ₃	1.872 B		
B ₂ B ₆	1.888 B		
B ₄ B ₅	1.716 B		
B ₅ B ₆	1.698 B		
B ₂ C	1.599 B		
B ₄ C	1.633 B		

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 B₂B₃B₆ 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).

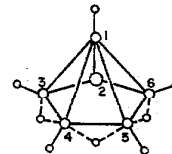
Methylphosphine-borane



CH ₃ BP		C _s	
Bond	Substitution	Angle	Substitution
CH _a	1.098 D	H _a BH _a	116.1 C
CH _s	1.087 B	H _s BH _s	112.3 C
BH _a	1.229 C	H _a CH _a	110.4 D
BH _s	1.234 C	H _s CH _s	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.

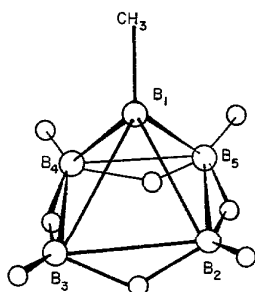
[1] P. S. Bryan and R. L. Kuczowski, *Inorg. Chem.* **11**, 553 (1972).

2-Carbahexaborane⁽⁹⁾

CH ₂ B ₅		C _s	
Bond	Substitution	Angle	Substitution
B ₃ B ₄	1.759 B	B ₃ B ₁ B ₄	59.11 C
B ₄ B ₅	1.830 B	B ₄ B ₁ B ₅	65.57 C
B ₁ B ₃	1.782 B	B ₃ B ₁ B ₅	103.9 C
B ₁ B 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 ₁ B ₂	1.687 C	1.62 X
B ₂ B ₃	1.800 C	
B ₁ C		

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

Trimethylphosphine-borane

CH ₁₂ BP		(CH ₃) ₃ P·BH ₃	C _{3v}
Bond	Substitution	Effective	Angle
PB		1.901 D	CPC
PC		1.819 D	HBH
BH	1.212 C		113.5 B
			105.0 D

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

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

Cyanogen iodide

CIN		ICN	C _{∞v}
Bond	Substitution	Effective	
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 _{∞v}
Bond	Effective	
N ... O	2.41 D	

Ground electronic state is ²Π₁.

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

Thiocyanogen

CNS	NCS	C _{∞v}
Bond	Effective	
N ... S	2.82 D	

Ground electronic state is ²Π₁.

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

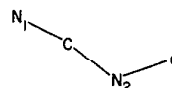
Cyanimidogen

CN ₂	NCN	D _{∞h}
Bond	Effective	
CN	1.232 A	

Ground electronic state is ³Σ_g⁻.

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

Nitrosyl cyanide

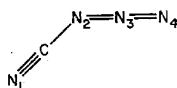


CN ₂ O		C _s	
Bond	Effective	Angle	Effective
N ₁ C	1.170 C	NCN	172.5 E
CN ₂	1.401 C	CNO	114.7 D
NO	1.228 C		

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 _{∞v}	
Bond	Substitution	Effective	Angle	Effective
CN ₂	1.164 B		CN ₂ N ₃ ^a	120.2 D
CN ₂ ^a		1.312 D	N ₁ CN ₃ ^a	176 E ^b
N ₂ N ₃ ^a		1.252 D		
N ₂ N ₄ ^a		1.153 D		

^a Derived with assumptions that N₂N₃N₄ linkage is linear and N₂N₄ is 1.133 ± 0.01 Å.

^b N₁ bent away from N₃ 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 _{∞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		OCS _e		C _{∞v}
Bond	Equilibrium	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 _{∞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 _{∞h}
Bond	Effective			
CO	1.177 A			

Ground electronic state is ²Π_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

CSS _e		SCS _e		C _{∞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

CST _e		TeCS		C _{∞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 _{∞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 _{∞h}
Bond	Effective		
CS	1.554 A		

Ground electronic state is ²I_g.

[1] J. H. Callomon, Proc. Roy. Soc. A244, 220 (1958).

C₂ Molecules

Chloriodoacetylene

C ₂ ClI		Cl-C≡C-I	C _{∞v}
Bond	Effective		
CC ^a	1.209		
CCI	1.627 D		
CI	1.989 D		

^a Assumed value.

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

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

C ₂ Cl ₃ F ₃		F ₃ C-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 ₂ Cl ₃ N		Cl ₃ CCN	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).

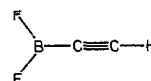
Trifluoroacetonitrile

C ₂ F ₃ N		CF ₃ CN	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).

Ethyldifluoroborane



C ₂ HBF 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 ₂ HBr		HC≡CBr	C _{∞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 ₂ HCl		HC≡CCl	C _{2v}
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 ₂ HF		HC≡CF	C _{2v}
Bond	Substitution		
CF	1.279 B		
CC	1.198 B		
CH	1.053 B		

Authors checked C₁ 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).

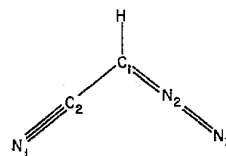
[2] J. K. Tyler and J. Sheridan, *Proc. Chem. Soc.* **1960**, 119.

Iodoacetylene

C ₂ HI		HC≡CI	C _{2v}
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 the CI distance.

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

Diazoacetonitrile

C ₂ HN ₃		C _s		
Bond	Substitution	Effective	Angle	Effective
C ₂ N ₁		1.165 X	C ₂ C ₁ N ₂	119.5 X
C ₂ C ₁		1.424 X	HC ₁ C ₂	117 X
C ₁ N ₂	1.280 C			
N ₂ N ₃		1.132 X		

Linearity of C₁N₂N₃ was assumed. CH bond assumed.

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

Acetylene

C ₂ H ₂		HC≡CH	D _{∞h}
Bond	Substitution	Equilibrium	
CII	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 ₂ H ₂ BrN		BrCH ₂ CN	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 ₂ H ₂ ClF		H ₂ C=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 ₂ H ₂ ClN		C ¹ H ₂ ClC ² N		C _s
Bond	Substitution	Angle	Substitution	
C ¹ Cl	1.781 X	C ² C ¹ Cl	111.5 X	
C ¹ H	1.088 X	C ² C ¹ H	107.5 X	

C¹C² and C²N bond lengths assumed. C¹C² assumed linear.

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

1,1-Difluoroethylene

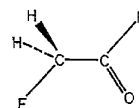
C ₂ H ₂ F ₂		H ₂ C=CF ₂		C _{2v}	
Bond	Substitution	Effective	Angle	Substitution	Effective
CC		1.315 D	HCH	121.1 C	
CH	1.074 C		FCF		109.0 D
CF		1.323 D			

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

cis 1,2-Difluoroethylene

C ₂ H ₂ F 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

C₂H₂F₂O C_s

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

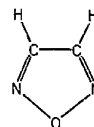
[1] E. Saegbarth and E. B. Wilson, Jr., *J. Chem. Phys.* **46**, 3088 (1967).

Hydrogen cyanide dimer

C₂H₂N₂ HCN ... HCN C_{∞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).

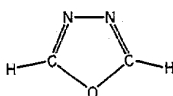
1,2,5-Oxadiazole

C₂H₂N₂O 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 D	CCN	109.0 A
CH	1.076 B	CCH	130.2 A

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

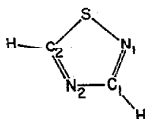
1,3,4-Oxadiazole

C₂H₂N₂OC_{2v}

Bond	Substitution	Angle	Substitution
CO	1.348 B	COC	102.0 C
CN	1.297 C	OCN	113.4 B
NN	1.899 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

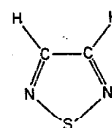
C₂H₂N₂SC_s

Bond	Substitution	Angle	Substitution
SN ₁	1.649 A	C ₂ SN ₁	92.8 A
N ₁ C ₁	1.317 A	SN ₁ C ₁	107.1 A
C ₁ N ₂	1.366 A	N ₁ C ₁ N ₂	120.1 A
N ₂ C ₂	1.313 A	C ₁ N ₂ C ₂	107.7 A
C ₂ S	1.707 A	N ₂ C ₂ S	112.3 A
C ₂ H	1.078 B	SC ₂ H	123.9 B
C ₁ H	1.078 (Assumed)	N ₂ C ₁ H	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).

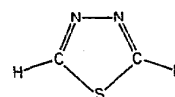
1,2,5-Thiadiazole

C₂H₂N₂SC_{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

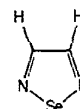
C₂H₂N₂SC_{2v}

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

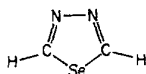
C₂H₂N₂SeC_{2v}

Planar molecule with C_{2v} symmetry established.

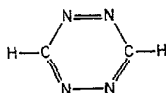
[1] G. L. Blackman, R. D. Brown, F. R. Burden, and J. E. Kent, *Chem. Phys. Lett.* **1**, 379 (1967).



1,3,4-Selenadiazole

C₂H₂N₂SeC_{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).

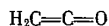
s-Tetrazine

C₂H₂N₄D_{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).

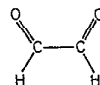
Ketene

C₂H₂OC_{2v}

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

[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] I. 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

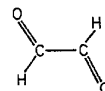
C₂H₂O₂C_{2v}

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).

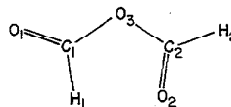
trans-Glyoxal

C₂H₂O₂C_{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).

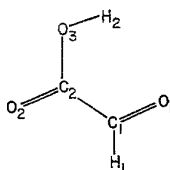
Formic anhydride

C₂H₂O₃C_s

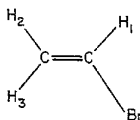
Bond	Substitution	Angle	Substitution
C ₁ O ₁	1.184 B	O ₁ C ₁ O ₃	120.6 B
C ₁ H ₁	1.101 B	H ₁ C ₁ O ₃	112.1 B
C ₁ O ₃	1.389 B	C ₁ O ₃ C ₂	117.8 B
C ₂ O ₃	1.364 A	H ₂ C ₂ O ₃	108.6 B
C ₂ O ₂	1.195 B	O ₂ C ₂ O ₃	126.1 B
C ₂ H ₂	1.096 D		

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

Glyoxylic acid

C₂H₂O₃ C_s

Bond	Substitution	Angle	Substitution
C ₁ O ₁	1.174 C	C ₂ C ₁ O ₁	123.7 C
C ₂ O ₂	1.203 C	C ₁ C ₂ O ₂	121.3 C
C ₂ O ₃	1.313 D	O ₂ C ₂ O ₃	126.2 C
C ₁ C 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 ₁ C ₂ O 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)C₂H₃Br 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).

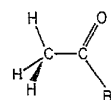
3-Methyl-3-bromodiazirine

C₂H₃BrN₂ Br(CH₃)C—N=N C_s

Bond	Effective
NN	1.240 C

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

Acetyl bromide

C₂H₃BrO 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 D	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).

Methylbromoforn

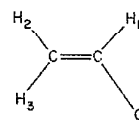
C₂H₃Br₃ H₃CCBr₂ C_{3v}

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)

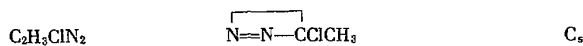
C₂H₃Cl C_s

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 CClCl 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).

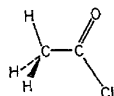
3-Methyl-3-chlorodiazirine
(Methylchlorodiazirine)



Bond	Effective
NN	1.241 C

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

Acetyl chloride



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

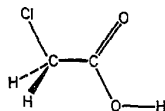
Methyl group has been assumed to be symmetrical.

^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).

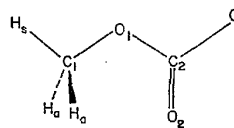
Chloroacetic acid



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



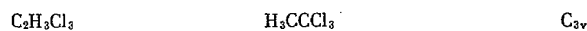
Bond	Substitution	Effective	Angle	Substitution	Effective
C ₂ Cl		1.73 D	ClC ₂ O ₂		126 D
C ₂ O ₁		1.36 D	O ₁ C ₂ O ₂		125 D
C ₁ O ₁		1.43 D	C ₁ O ₁ C ₂		115 D
C ₁ H _s	1.072 C		O ₁ C ₁ H _s		105 D
C ₁ H _a	1.076 C		O ₁ C ₁ H _a		110 D
			H _s C ₁ H _a	111.1 C	
			H _s C ₁ H _a	110.4 C	

The effective parameters were calculated under the assumption that the C₂O₂ 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



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. Daring, 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 ₂ H ₃ F			C _s		
Bond	Substitution	Effective	Angle	Substitution	Effective
C ₁ C ₂ ^a		1.329 D	FCC		120.8 D
C ₁ F		1.347 D	FCH ₁		110.0 F
C ₁ H ₁		1.082 D	H ₂ CC ^a		120.9 D
C ₂ H ₂	1.087 C		H ₃ CC ^a		119.0 D
C ₂ H ₃	1.077 C		H ₃ C ₂ H ₂	120.1 C	

^a These parameters are near-substitution values. All coordinates except one coordinate of C₁ are substitution values.

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

Acetyl Fluoride

C ₂ H ₃ FO		CH ₃ COF		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 ₁	110.4 E		
CH ₁	1.082 C	CCH ₂	108.8 E		
CH ₂	1.096 C	H ₁ CH ₁	110.8 E		
		H ₁ CH ₂	107.3 E		

H₁ and H₂ refer to in plane and out of plane hydrogens. The oxygen atom eclipses a methyl hydrogen.

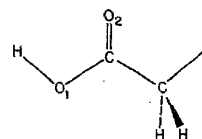
[1] L. Pierce and L. C. Krisher, *J. Chem. Phys.* **31**, 875 (1959).

cis-Fluoroacetic acid

C ₂ H ₃ FO ₂		CH ₂ FCO ₂ H		C _s	
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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 ₂ H ₃ FO ₂		C _s	
Bond	Substitution		
O ₁ H		0.973 C	
O ₁ O ₂ ^a		2.258 A	
O ₂ H ^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, G. van der Plaats and P. H. van Roon, *J. Mol. Struct.* **11**, 67 (1972).

1,1,2-Trifluoroethane

C ₂ H ₃ F ₃		HF ₂ C-CH ₂ F		C ₁	
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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 ₂ H ₃ N		CH ₃ CN		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).

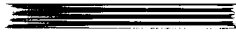
[2] C. Matsumura, E. Hirota, T. Oka, and Y. Morino, *J. Mol. Spectrosc.* **9**, 366 (1962).

Acetonitrile-N-oxide

C ₂ H ₃ NO		H ₃ C-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. Bodensch and K. Morgenstern, *Z. Naturforsch. A* **25**, 150 (1970).

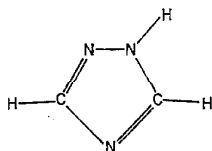


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Nitroethylene $C_2H_3NO_2$ $H_2C=CHNO_2$ C_s

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 Lerberghe, 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 $ClCH_2-CH_2F$ 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

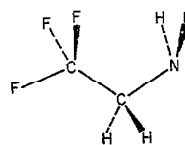
Microwave data showed that the heavy atom skeleton and the amino hydrogens lie in a plane, and that the C=O and C-F bonds were in the *trans* conformation.

- [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.

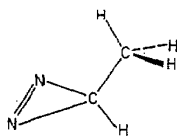
- [1] E. C. Thomas and V. W. Laurie, J. Chem. Phys. **44**, 2602 (1966).

Amino acetonitrile $C_2H_4N_2$ H_2N-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

C₂H₄N₂C_s

Distance	Substitution	Effective
NN		1.235 C
H ₁ H ₂ ^a	1.771 B	

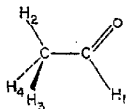
The equilibrium orientation of the methyl group is staggered.

^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

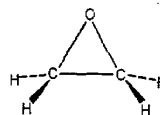
C₂H₄OC_s

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 ₃ CH ₁	108.9 C	108.7 C

The effective parameters were recalculated from reported data. The CCH₁ 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)C₂H₄OC_{2v}

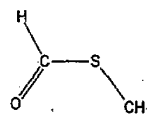
Bond	Substitution	Effective	Angle	Substitution	Effective
CC	1.466 B	1.470 B	HCH	116.6 B	116.3 D
CO	1.431 B	1.434 B	θ ^a	22.0 B	22.3 B
CH	1.085 B	1.085 B			

^a Angle between CC bond and the line which bisects the HCH angle.

[1] C. Hirose, *Bull. Chem. Soc. Japan* **47**, 1311 (1974).

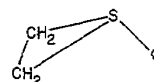
[2] G. L. Cunningham, A. W. Boyd, R. J. Myers and W. D. Gwinn, *J. Chem. Phys.* **19**, 676 (1951).

Methyl thioformate

C₂H₄OSC_s

Microwave data are consistent with a *cis* conformation.

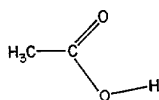
[1] G. I. L. Jones, D. G. Lister, N. L. Owen, M. C. L. Gerry and P. Palmieri, *J. Mol. Spectrosc.* **60**, 348 (1976).

Thiirane-1-oxide
(Ethylene episulfoxide)C₂H₄OSC_s

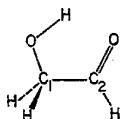
Bond	Effective	Angle	Effective
SO	1.483 D	OSC	110.0 D
CS	1.822 D	CSC	48.8 D
CC	1.504 D		

Assumptions: CH = 1.078, HCH = 116.0, HCC = 151.7.

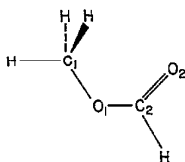
[1] S. Saito, *Bull. Chem. Soc. Japan* **42**, 663 (1969).

Acetic acidC₂H₄O₂C_s

Microwave data are consistent only with the above conformation.

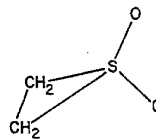
[1] I. C. Krisher and E. Saegbarth, *J. Chem. Phys.* **54**, 4553 (1971).[2] W. J. Tabor, *J. Chem. Phys.* **27**, 974 (1957).**Glycolaldehyde**C₂H₄O₂C_s

Bond	Substitution	Angle	Substitution
C ₂ O	1.209 A	C ₁ C ₂ O	122.7 B
C ₁ O	1.437 B	C ₂ C ₁ O	111.5 B
CC	1.499 A	C ₁ C ₂ H	115.3 B
OH	1.051 B	C ₂ C ₁ H	109.2 B
C ₂ H	1.102 B	C ₁ OII	101.6 B
C ₁ H	1.093 B	HC ₁ H	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**C₂H₄O₂C_s

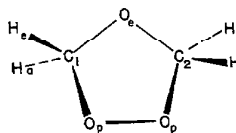
Bond	Substitution	Angle	Substitution
C ₂ O ₂	1.200 B	O ₁ C ₂ O ₂	125.9 B
C ₂ O ₁	1.334 B	C ₁ O ₁ C ₂	114.8 B
C ₁ O ₁	1.437 B	HC ₂ O ₁	109.3 B
C ₂ H	1.101 B	HC ₁ H	110.7 C
C ₁ H	1.086 C		

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)**C₂H₄O₂SC_{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		

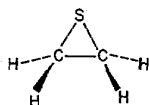
Assumptions: CH = 1.078, HCH = 116.0, HCC = 151.7.

[1] Y. Nakano, S. Saito and Y. Morino, *Bull. Chem. Soc. Japan* **43**, 368 (1970).**1,2,4 Trioxolane
(Ethylene ozonide)**C₂H₄O₃C₂

Bond	Substitution	Angle	Substitution	Dihed. Angle	Substitution
CH _a	1.091 C	COC	104.8 B	C ₁ O _a C ₂ O _p	-16.2 B
CH _b	1.097 C	COO	99.3 B	C ₁ O _p O _p C ₂	-49.5 B
CO _a	1.416 B	OCO	105.5 B	O _a CO _p O _p	40.8 B
CO _p	1.412 B	HCH	113.3 C	C ₁ O _a C ₂ H _a	-131.3 C
O _p O _p	1.461 B	O _a CH _a	110.8 C	C ₁ O _a C ₂ H _a	102.8 C
		O _a CH _b	109.8 C		
		O _p CH _a	106.7 C		
		O _p CH _b	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)



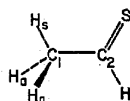
C_2H_4S C_{2v}

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	$C_2C_1H_5$	111.2 C
C_1H_6	1.090 C	$C_2C_1H^a$	110.1 C
C_1H_7	1.098 D		

- [1] H. W. Kroto and B. M. Landsberg, *J. Mol. Spectrosc.* **62**, 346 (1976).

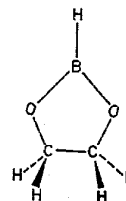
Ethynylsilane (Silyl Acetylene)

C_2H_4Si C_{3v} $H_3SiC\equiv CH$

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. Muentner and V. W. Laurie, *J. Chem. Phys.* **39**, 1181 (1963).

1,3,2-Dioxaborolane



$C_2H_6BO_2$ C_2

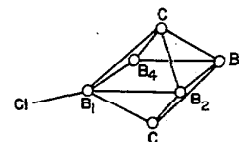
Bond	Substitution	Effective	Angle	Substitution	Effective
CC	1.541 B		OBO		114.2 D
CO		1.438 D	BOC		107.3 D
BO		1.368 D	OCC		104.9 D
CH		1.093 D	HCH		109.2 D
BH	1.20	(assumed)	HCC		112.5 D
			α^a		11.8
			β^b		7.1

^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-dicarbaborane (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 ₂ H ₅ Br		H ₃ C-C ² H ₂ Br		C _s
Bond	Substitution	Angle	Substitution	
CBr	1.950 C	CCBr	111.0 C	
CC	1.518 B	C ¹ C ² H	112.2 C	
C ¹ H	1.093 C	HC ² H	109.9 C	
C ² H	1.087 C	HC ¹ H	108.9 C	

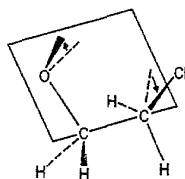
Methyl group was assumed to be symmetrical.
[1] C. Flanagan and L. Pierce, J. Chem. Phys. **38**, 2963 (1963).

Chloroethane
(Ethyl chloride)

C ₂ H ₅ Cl		CH ₃ CH ₂ Cl		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. CH₃ 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 ₂ H ₅ ClO				C _s
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...H ₁	2.609 B	(CCO)-(COH ₁) ^b	58.4 X	

^a Assumed value.

^b Dihedral angles between indicated planes.

[1] R. C. Azrak and E. B. Wilson, J. Chem. Phys. **52**, 5299 (1970).

Fluoroethane

C ₂ H ₅ F		CH ₃ CH ₂ F		C _s
Bond	Substitution Effective	Angle	Substitution Effective	
CC	1.505 B	H _g CH _g	108.9 B	
CF	1.398 B	H _g CH _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).

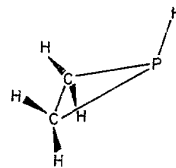
Nitroethane

C ₂ H ₅ NO ₂		CH ₃ CH ₂ NO ₂		C _s
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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 ₂ H ₅ P				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).

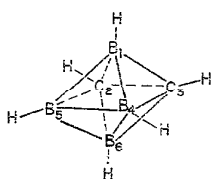
Methyl isocyanide-borane

C ₂ H ₃ BN		C ¹ H ₃ NC ² -BH ₃		C _{2v}
Bond	Substitution	Angle	Effective	
C ¹ N	1.416 B	HCH	110.0 C	
NC ²	1.155 C	HBH	113.0 C	
C ² B	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. Coanangel and M. Grace Hu, J. Amer. Chem. Soc. **99**, 1442 (1977).

1,2-Dicarbaborane (6)



C ₂ H ₆ B ₄		C _{2v}	
Bond	Substitution	Bond	Substitution
B ₁ B ₂	2.434 B	B ₄ C ₃	1.605 B
C ₂ B ₄	2.297 B	C ₂ C ₃	1.540 B
B ₁ B ₃	1.721 D	B ₁ C ₂	1.627 D
B ₁ B ₄	1.752 B		

[1] R. A. Baudet and R. L. Poynter, J. Chem. Phys. **53**, 1899 (1970).

Dimethylcadmium

C ₂ H ₆ Cd		CH ₃ CdCH 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, E. P. Stoicheff and R. Turner, Can. J. Phys. **38**, 1516 (1960).

Vinylgermane

C ₂ H ₆ Ge		H ₂ C=CH-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. Daring, K. L. Kizer and Y. S. Li, J. Amer. Chem. Soc. **96**, 7400 (1974).

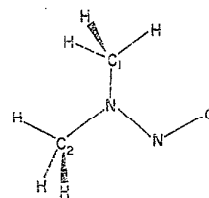
Dimethylmercury

C ₂ H ₆ Hg		CH ₃ HgCH 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 CH₃C 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 ₂ H ₆ N ₂ O		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.

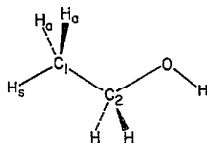
[1] A. Guarnieri, F. Rohwer and F. Scappini, Z. Naturforsch. **30a**, 904 (1975).

[2] F. Scappini, A. Guarnieri, H. Dreizler and P. Rademacher, Z. Naturforsch. **27a**, 1529 (1972).

gauche-EthanolC₂H₆OC₁

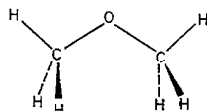
This conformer has OH group rotated 126° (X) from the well-established *trans* position.

[1] Y. Sasada, *J. Mol. Spectrosc.* **38**, 33 (1971).

trans-EthanolC₂H₆OC_{2v}

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 ₁ C ₂ H	110.7 B
C ₂ H	1.098 B	HC ₂ H	108.0 D
C ₁ H _a	1.091 C	C ₂ C ₁ H _a	110.1 B
C ₁ H _b	1.088 C	C ₂ C ₁ H _b	110.5 C
		H _a C ₁ H _a	108.4 B

[1] J. P. Culot, Fourth Austin Symposium on Gas Phase Molecular Structure, Paper T8 (1972).

Methyl EtherC₂H₆OC_{2v}

Bond	Substitution	Angle	Substitution
CO	1.410 B	COC	111.7 B
CH _a	1.100 B	OCH _a	110.8 B
CH _b	1.091 C	OCH _b	107.2 C
		H _a CH _a	108.7 B
		H _b CH _b	109.5 C

Hydrogens s and a are in and out of the heavy atom plane, respectively.

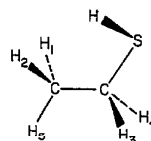
[1] U. Blukis, P. H. Kasai, and R. J. Myers, *J. Chem. Phys.* **38**, 2753 (1963).

Methyl SulfoxideC₂H₆OS(CH₃)₂SOC_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 C₃ axis along the CS bond.

[1] H. Dreizler and G. Dendl, *Z. Naturforsch.* **19a**, 512 (1964).

gauche-EthaneithiolC₂H₆SC₁

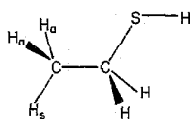
Bond	Effective	Angle	Effective
SH	1.336 C	HSC	96.0 C
SC	1.814 C	CCS	113.6 C
CH ₄	1.089 D	H ₁ CH ₂	106.6 D
CH ₃			
CC	1.528 C	H ₄ CC	110.7 D
CH ₅		H ₃ CC	111.3 D
CH ₁	1.091 D	H ₄ CS	104.9 D
CH ₂		H ₃ CS	109.3 D
		CCH ₅	110.5 D
		CCH ₁	110.6 D
		H ₅ CH ₁	109.0 D
		H ₁ CH ₂	106.9 D

Assumed: CH₃ = CH₄, CH₁ = CH₂, CH₅ = CH₁, and H₅H₁ = H₅H₂.

[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 ₂ H ₆ S		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 _b	1.095 C	CCH _a	109.7 C
		CCH _b	110.6 B
		H _a CH _a	108.9 C
		H _b CH _b	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 ₂ H ₆ S		CH ₃ SCH ₃		C _{2v}
Bond	Substitution	Angle	Substitution	
CS	1.802 A	CSC	98.87 A	
CH _a	1.091 A	H _a CH _a	109.5 A	
CH _b	1.091 E	H _b CH _b	109.6 E	
		SCH _a	110.75 A	
		SCH _b	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. Driezler and H. D. Rudolph, *Z. Naturforsch.* **17a**, 712 (1962).

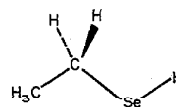
Dimethyl Disulfide

C ₂ H ₆ S ₂		CH ₃ SSCH 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 C₃ 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 ₂ H ₆ Se			C _s	
Bond	Substitution	Effective	Angle	Effective
CC		1.543 C	CCSe	108.8 C
CS _c		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).

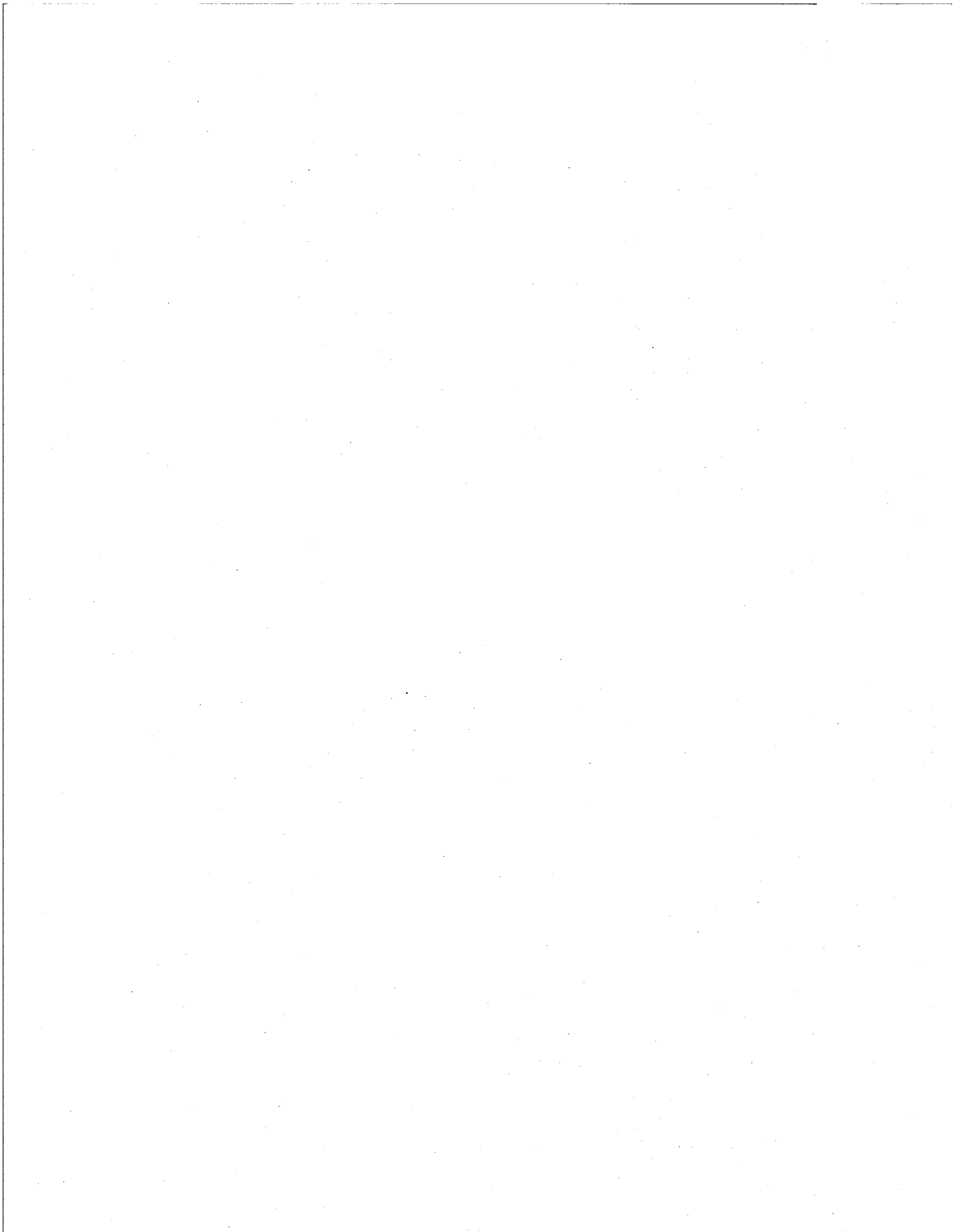
- [1] J. R. Durig and W. E. Bucy, *J. Mol. Spectrosc.* **64**, 474 (1977).

Methyl Selenide

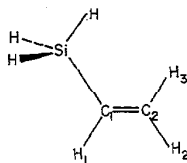
C ₂ H ₆ Se		CH ₃ SeCH ₃		C _{2v}	
Bond	Substitution	Effective	Angle	Substitution	Effective
SeC	1.943 B		CSeC	96.2 B	
CH		1.093 C	SeCH _a		109.6 C
			SeCH _b		106.7 C
			HCH		110.3 C

Methyl groups assumed symmetric.

- [1] J. F. Beecher, *J. Mol. Spectrosc.* **4**, 414 (1966).



Vinylsilane

C₂H₅Si 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 ₂ C ₁ H ₁	118.0 B	
C ₁ H ₁	1.094 B		C ₁ C ₂ H ₂		120.6 X
C ₂ H ₂	1.097 B		C ₁ C ₂ H ₃	120.3 B	

The C₂H₂ distance was assumed to be equal to the C₂H₃ distance. The SiH₃ group was assumed to be symmetric. The axis of the SiH₃ group is tilted 1.8° toward the methylene group.

[1] J. M. O'Reilly and L. Pierce, J. Chem. Phys. **34**, 1176 (1961).

Dimethylzinc

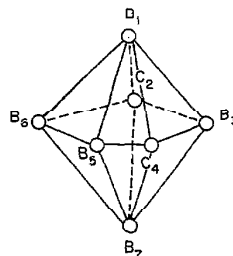
C₂H₆Zn CH₃ZnCH₃ Undetermined

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)

C₂H₇B₅ C_{2v}

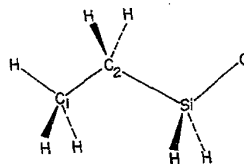
Bond	Substitution	Angle	Substitution
C ₂ B ₆	1.563 B	C ₂ B ₃ C ₄	99.9 B
C ₂ B ₃	1.546 B	B ₃ C ₄ B ₅	116.8 A
C ₂ B ₁	1.708 B	C ₄ B ₅ B ₆	103.2 A
B ₅ B ₆	1.651 B	C ₂ B ₃ B ₇	79.7 C
B ₁ B ₅	1.815 D		
B ₁ B ₃	1.818 D		

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

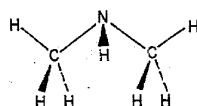
C₂H₇ClSi C_s

Bond	Effective	Angle	Effective
SiCl	2.060 X	C ₂ SiCl	109.9 X
SiH	1.478 X	C ₂ SiH	113.6 X
SiC ₂	1.869 X	SiC ₂ H	105.6 X
C ₁ C ₂	1.532 X	C ₂ C ₁ H	111.9 X
C ₂ H	1.107 X	C ₁ C ₂ Si	111.3 X
C ₁ H	1.082 X	α ₁	117.7 X
		α ₂	121.8 X

α₁ is the angle between the CCSi plane and the CSiH plane and α₂ is the angle between the CCSi plane and the SiCH plane. A *gauche* form exists also, with C₁C₂Si = 113.0 (X) and the SiH₂Cl group rotated by 120.4° (X).

[1] V. Typke, M. Dakkouri and W. Zeil, Z. Naturforsch. **29a**, 1081 (1974).

Dimethylamine

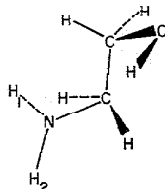
C₂H₇NC_s

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

C₂H₇NOC_i

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

C₂H₇PCH₃CH₂PH₂

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

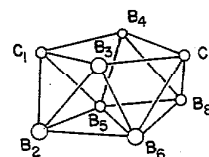
C₂H₇P(CH₃)₂PHC_s

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 CH₃ 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)

C₂H₈B₆C_s

Bond	Substitution	Angle	Substitution
B ₂ B ₃	1.813 C	B ₂ B ₃ B ₆	52.7 B
B ₂ B ₅	1.843 C	B ₅ B ₂ B ₆	66.9 C
B ₂ B ₆	1.685 C	B ₂ B ₆ B ₃	60.4 C
B ₃ B ₄	1.886 C	B ₂ B ₃ B ₆	54.3 B
B ₅ B ₆	1.880 C	B ₂ B ₆ B ₃	60.8 B
B ₆ B ₆	1.949 C	B ₃ B ₂ B ₆	64.9 B

[1] H. N. Rogers, K. Lau and R. A. Beaudet, *Inorg. Chem.* **15**, 1775 (1976).

Dimethylgermane

C₂H₆Ge(CH₃)₂GeH₂C_{2v}

Bond	Effective	Angle	Effective
GeC	1.95 C	CGeC	110 C

CH and HCH parameters assumed from CH₃GeH₃.

[1] E. C. Thomas and V. W. Laurie, *J. Chem. Phys.* **50**, 3512 (1969).

Ethylermane

$\text{H}_3\text{C}^{(2)}\text{C}^{(2)}\text{H}_2\text{GeH}_3$			
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
$\text{C}^{(2)}\text{H}$	1.093 C	$\text{HC}^{(2)}\text{H}$	106.4 C
$\text{C}^{(1)}\text{H}$	1.091 C	$\text{GeC}^{(2)}\text{H}$	111.6 C
		$\text{C}^{(2)}\text{C}^{(1)}\text{H}$	110.9 C
		$\text{HC}^{(1)}\text{H}$	108.0 C

Methyl and germyl groups were assumed to be symmetrical.

[1] J. R. Daring, A. D. Lopata and P. Groner, *J. Chem. Phys.* **66**, 1888 (1977).

Dimethylsilane

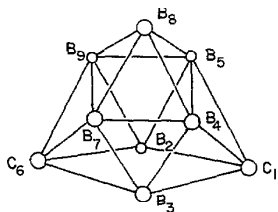
$(\text{CH}_3)_2\text{SiH}_2$			
Bond	Substitution	Angle	Substitution
SiC	1.867 A	CSiC	110.98 A
SiH	1.483 B	HSiH	107.83 B
CH	1.095 B	HCH	108.00 B
		θ^a	110.83 B

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).

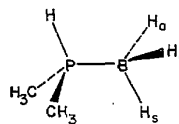
1,6-Dicarbanonaborane (9)



$\text{C}_2\text{H}_3\text{B}_7$	
Bond	Substitution
B_6B_5	1.712 C
B_5B_3	1.995 B
B_3B_4	1.976 C
B_7B_3	1.784 B
B_2B_3	1.805 B

[1] K. Lau and R. A. Beaudet, *Inorg. Chem.* **15**, 1059 (1976).

Dimethylphosphine-borane



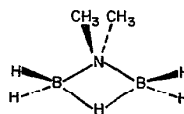
$\text{C}_2\text{H}_{10}\text{BP}$					
Bond	Substitution	Effective	Angle	Substitution	Effective
BH_a	1.216 C		PBH_a	104.8 C	
BH_b	1.212 C		PBH_b	104.9 C	
PB		1.898 D	CPB		114.6 D
PC		1.813 D	CPC		105.4 D
PH		1.414 D	BPH		118.1 X

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)



$\text{C}_2\text{H}_{11}\text{B}_2\text{N}$					
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 ₂ BrCl		ClC≡CBr		C _{∞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 ₂ N		CNC		D _{∞h}	
Bond		Effective			
CN		1.245 A			

Ground electronic state is ²Π_g.

[1] A. J. Merer and D. N. Travis, *Can. J. Phys.* **44**, 353 (1966).

Cyanomethylidyne

C ₂ N		CCN		C _{∞v}	
Bond		Effective			
C...N		2.56 D			

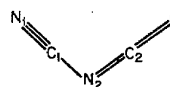
Ground electronic state is ²Π_g.

[1] A. J. Merer and D. N. Travis, *Can. J. Phys.* **43**, 1795 (1965).

Cyanogen

C ₂ N ₂		N≡C—C≡N		D _{∞h}	
Bond		Effective			
CC		1.389 E			
CN		1.154 D			

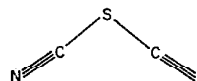
[1] A. G. Maki, *J. Chem. Phys.* **43**, 3193 (1965).

Cyanogen Isocyanate

C ₂ N ₂ O				C _s	
Bond		Effective		Angle	
N ₁ C ₁		1.164 ^a		NCN	
N ₂ C ₂		1.218 ^a		NCO	
CO		1.165 ^a		CNC	
C ₁ N ₂		1.283 X		180 ^a	
				180 ^a	
				140 X	

^a Assumed values.

[1] W. H. Hocking and M. C. L. Gerry, *J. Mol. Spectrosc.* **59**, 338 (1976).

Sulfur Cyanide

C ₂ N ₂ S				C _{2v}	
Bond		Substitution		Angle	
SC		1.701 B		CSC	
CN		1.156 B		SCN	
				98.3 B	
				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 ₂ O		CCO		C _{∞v}	
Bond		Effective			
C...O		2.52 D			

Ground electronic state is ²Σ⁻.

[1] C. Devillers and D. A. Ramsay, *Can. J. Phys.* **49**, 2839 (1971).

C₃ Molecules**Tricarbon (Propadiene-1,3-diyldene)**

C ₃		CCC	D _{∞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 ₃ BrN		Br—C ¹ ≡C ² —C ³ ≡N	C _{∞v}
Bond	Substitution		
CBr	1.786 B		
C ¹ C ²	1.204 B		
C ² C ³	1.370 A		
CN	1.159 A		

[1] T. Bjorvatten, *J. Mol. Struct.* **20**, 75 (1974).**1-Chloro-3,3,3-Trifluoropropyne**

C ₂ CF ₃		F ₃ C ¹ C ² ≡C ³ Cl	C _{3v}
Bond	Substitution	Effective ^a	
C ³ Cl	1.629 C	1.627 C	
C ¹ ...C ³	2.647 B		
C ¹ C ²		1.453 C	
C ² C ³		1.199 C	
CF		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**

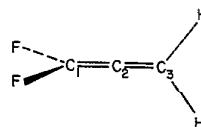
C ₃ ClN		Cl—C ¹ ≡C ² —C ³ ≡N	C _{∞v}
Bond	Substitution		
CCl	1.625 B		
C ¹ C ²	1.209 B		
C ² C ³	1.369 B		
CN	1.160 A		

[1] T. Bjorvatten, *J. Mol. Struct.* **20**, 75 (1974).**3,3,3-Trifluoro-1-Propyne**

C ₃ HF 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**

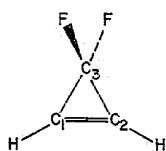
C ₃ HN		HCCCN	C _{∞v}
Bond	Substitution	Effective	
CH	1.058 A	1.057 A	
C≡C	1.205 A	1.203 A	
C—C	1.378 A	1.382 A	
CN	1.159 A	1.157 A	

[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 ₃ H ₂ F ₂		C _{2v}			
Bond	Effective	Substitution	Angle	Effective	Substitution
C ₂ C ₃		1.306 B	HCH		117.8 B
CH		1.086 B	CCH		121.1 B
C ₁ C 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 ₃ H ₂ F ₂			C _{2v}		
Bond	Substitution	Effective	Angle	Substitution	Effective
C ₁ C ₂	1.321 A		FCF		105.5 D
CH	1.075 A		C ₁ C ₃ C ₂		54.6 C
C ₁ C ₃		1.438 C	HC ₁ C 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

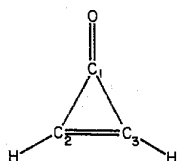
C ₃ H ₂ N ₂		CH ₂ (CN) ₂		C _{2v}	
Bond	Effective	Angle	Effective		
CC	1.47 E	CCC	109 E		
CN	1.17 E	HCH	109 E		
CH	1.09 D	CCN ^a	174 E		

^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).

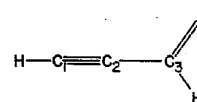
Cyclopropenone



C ₃ H ₂ O		C _{2v}	
Bond	Substitution	Angle	Substitution
CO	1.212 B	HC ₂ C ₃	144.9 B
C ₁ C ₂	1.412 C	C ₂ C ₃ C ₁	62.6 B
C ₂ C 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 ₃ H ₂ O			C _s		
Bond	Substitution	Average	Angle	Substitution	Average
HC ₁	1.055 B	1.054 C	C ₂ C ₃ O	123.9 D	124.2 B
HC ₃	1.106 B	1.114 C	C ₂ C ₃ H	113.9 D	113.8 D
C ₁ C ₂	1.209 B	1.205 C	C ₁ C ₂ C ₃	178.4 E ^a	178.6 C
C ₂ C ₃	1.444 B	1.449 A	HC ₁ C ₂	180.0 E	
C ₃ O	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).

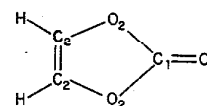
Propiolic Acid
(Propargylic or Propynoic Acid)

C ₃ H ₂ O ₂	HC≡CCOOH	C _s
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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 ₃ H ₂ O ₃		C _{2v}	
Bond	Substitution	Angle	Substitution
C ₂ C ₂	1.331 A	C ₂ C ₂ O ₂	108.6 X
C ₂ O ₂	1.385 X	C ₂ O ₂ C ₁	106.9 X
C ₁ O ₂	1.364 X	O ₂ C ₁ O ₂	108.8 X
C ₁ O ₁	1.191 A		

[1] W. F. White and J. E. Boggs, J. Chem. Phys. **54**, 4714 (1971).

3-Bromopropyne
(Propargyl bromide)

C ₃ H ₃ Br		BrH ₂ C ³ C ² ≡C ¹ H		C _s
Bond	Effective	Angle	Effective	
C ³ Br	1.94 E	C ² C ³ Br	112 E	
C ² C ³	1.46 E			

Four isotopic species studied; C¹H, C³H, C²≡C¹ and C²C³H values were assumed.

[1] Y. Kikuchi, E. Hirota and Y. Morino, Bull. Chem. Soc. Japan **34**, 348 (1961).

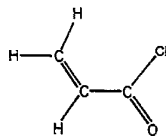
3-Chloropropyne
(Propargyl Chloride)

C ₃ H ₃ Cl		ClH ₂ C ³ C ² ≡C ¹ H		C _s
Bond	Effective	Angle	Effective	
CCl	1.780 E	CCCl	111.9 E	
C ² C ³	1.465 E	HCH	108.7 D	
		C ² C ³ H	111.5 E	

Four isotopic species studied; C¹H, C³H, C²≡C¹ bond lengths were assumed.

[1] E. Hirota and Y. Morino, Bull. Chem. Soc. Japan **34**, 341 (1961).

trans-Propenoyl Chloride
(trans-Acryloyl Chloride)

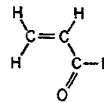


C₃H₃ClO C_s

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)



C₃H₃FO 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.

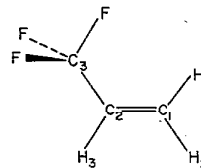
[1] J. J. Keirns and R. F. Curl, Jr., J. Chem. Phys. **48**, 3773 (1968).

cis-1,2,3-Trifluorocyclopropane

C ₃ H ₃ F 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



C₃H₃F₃ C_s

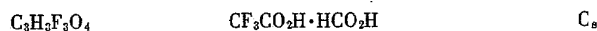
Bond	Effective	Angle	Effective
C ₂ C ₃	1.489 B	FCF	106.8 C
C ₁ C ₂	1.312 C	C ₃ C ₂ C ₁	124.8 C
CH ₁	1.085 C	CCH ₁	120.6 D
CH ₂	1.092 C	CCH ₂	122.8 D
CH ₃	1.109 B	C ₁ C ₂ H ₃	121.2 D
CF ^a	1.345 B	θ ^b	1.0 D

^a Assumed value.

^b Tilt angle of the CF₃ 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).

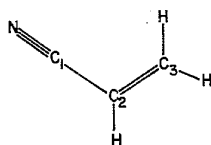
Trifluoroacetic Acid-Formic Acid Dimer



Bond	Effective
O...O	2.67 X

[1] C. C. Costain and G. P. Srivastava, *J. Chem. Phys.* **41**, 1620 (1964).

Vinyl cyanide

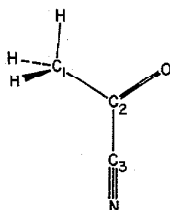


Bond	Substitution	Angle	Substitution
CN	1.164 B	C ₁ C ₂ C ₃	122.6 C
C ₁ C ₂	1.426 B	HC ₂ C ₃	121.7 B
C ₂ C ₃	1.339 B		
C ₂ H	1.086 B		

C₂C₁N was linear to within experimental accuracy.

[1] C. C. Costain and B. P. Stoicheff, *J. Chem. Phys.* **30**, 777 (1959).

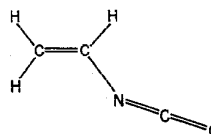
Acetyl cyanide



Bond	Substitution	Effective	Angle	Substitution	Effective
CO	1.226 D		C ₁ C ₂ O	124.0 D	
C ₁ C ₂	1.490 D		C ₁ C ₂ C ₃	115.0 D	
C ₂ C ₃	1.466 C		HCH	108.7 C	
CN	1.164 C				
CH		1.086 C			

C₂C₃N group was assumed to be linear, and the methyl group was assumed to be symmetrical.

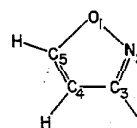
[1] L. C. Krisher and E. B. Wilson, *J. Chem. Phys.*, **31**, 882 (1959).

Isocyanoethene
(Vinyl isocyanate)

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

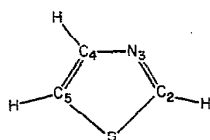


Bond	Substitution	Angle	Substitution
O ₁ N ₂	1.399 A	C ₅ O ₁ N ₂	108.9 A
N ₂ C ₃	1.308 A	O ₁ N ₂ C ₃	105.3 A
C ₃ C ₄	1.426 A	N ₂ C ₃ C ₄	112.3 A
C ₄ C ₅	1.357 A	C ₃ C ₄ C ₅	103.0 A
C ₅ O ₁	1.344 A	C ₄ C ₅ O ₁	110.5 A
C ₃ H	1.078 B	C ₄ C ₃ H	129.1 B
C ₄ H	1.074 B	C ₅ C ₄ H	128.5 B
C ₅ H	1.074 B	C ₄ C ₅ H	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

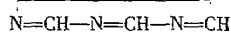
C₂H₃NSC_s

Bond	Substitution	Angle	Substitution
SC ₂	1.724 X	C ₃ SC ₂	89.3 X
C ₂ N	1.304 X	SC ₂ N	115.1 X
NC ₄	1.372 A	C ₂ NC ₄	110.1 X
C ₄ C ₅	1.367 X	NC ₄ C ₅	115.8 X
C ₅ S	1.713 X	C ₄ C ₅ S	109.5 X
C ₂ H ₂	1.077 X	SC ₂ H ₂	121.2 X
C ₄ H ₄	1.080 A	NC ₄ H ₂	123.5 X
C ₅ H ₅	1.076 X	NC ₄ H ₄	119.3 A
		C ₃ C ₄ H ₄	124.8 X
		C ₄ C ₅ H ₅	129.0 X
		SC ₃ H 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

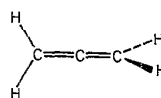
C₃H₃N₃D_{3h}

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).

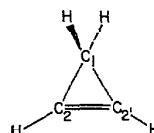
Allene

C₃H₄D_{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).

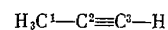
Cyclopropene

C₃H₄C_{2v}

Bond	Substitution	Angle	Substitution
C ₁ C ₂	1.509 B	C ₁ C ₂ C _{2'}	50.8 A
C ₂ C _{2'}	1.296 A	C ₂ C _{2'} H	149.9 B
C ₂ H	1.072 B	HCH	114.6 B
C ₁ H	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

C₃H₄C_{3v}

Bond	Substitution	Angle	Substitution
C ¹ C ²	1.459 B	HC ¹ C ²	110.2 B
C ² C ³	1.206 B		
C ² H	1.056 B		
C ¹ H	1.105 B		

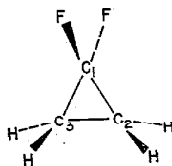
- [1] C. C. Costain, *J. Chem. Phys.* **29**, 864 (1958).
 [2] R. Trambarulo and W. Gordy, *J. Chem. Phys.* **18**, 1613 (1950).
 [3] L. F. Thomas, E. I. Sherrard and J. Sheridan, *Trans. Faraday Soc.* **51**, 619 (1955).

1,1-Dichlorocyclopropane

$\text{Cl}_2\text{C}^1-\text{C}^2\text{H}_2-\text{C}^3\text{H}_2$

Bond	Substitution	Angle	Substitution
CH	1.085 B	HCH	117.5 B
C ² C ³	1.534 B	C ² C ³ H	117.5 B
C ¹ C ²	1.532 C	ClCCl	114.2 C
CCl	1.734 C	C ² C ³ C ¹	60.1 B

[1] W. H. Flygare, A. Narath, and W. D. Gwinn, *J. Chem. Phys.* **36**, 200 (1962).

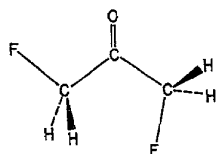
1,1-Difluorocyclopropane

$\text{C}_3\text{H}_4\text{F}_2$

Bond	Substitution	Angle	Substitution
C ₁ C ₂	1.464 C	FCF	108.3 C
C ₂ C ₃	1.553 A	HCH	116.9 B
CF	1.355 C		
CH	1.082 B		

Structural parameters were evaluated for the D₄ species.

[1] A. T. Perretta and V. W. Laurie, *J. Chem. Phys.* **62**, 2469 (1975).

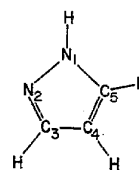
1,3-Difluoroacetone

$\text{C}_3\text{H}_4\text{F}_2\text{O}$

Bond	Substitution	Effective	Angle	Substitution	Effective
CO	1.219 C		CCO	123.3 C	
C ₁ C ₂	1.470 B		C ₂ C ₁ H	115.1 B	
C ₁ H	1.108 B		C ₁ C ₂ H	117.3 B	
C ₂ H	1.084 B		C ₁ C ₂ C ₃		119.8 C
C ₂ C ₃		1.345 B	C ₂ C ₃ H ₁		121.5 C
C ₃ H ₁		1.086 C	C ₂ C ₃ H ₂		120.0 C
C ₃ H ₂		1.086 C			

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.

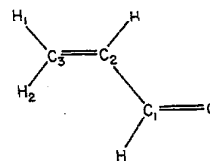
[1] D. J. Finnigan, C. W. Cillies, R. D. Suenram and E. B. Wilson, *J. Mol. Spectrosc.* **57**, 363 (1975).

Pyrazole

$\text{C}_3\text{H}_4\text{N}_2$

Bond	Substitution	Angle	Substitution
N ₁ N ₂	1.349 B	N ₁ N ₂ C ₃	104.1 B
N ₂ C ₃	1.331 B	N ₂ C ₃ C ₄	111.9 B
C ₃ C ₄	1.416 B	C ₃ C ₄ C ₅	104.5 B
C ₄ C ₅	1.372 A	C ₄ C ₅ N ₁	106.4 B
C ₅ N ₁	1.359 B	C ₅ N ₁ N ₂	113.1 B
N ₁ H	0.998 B	N ₂ C ₃ H	119.3 B
C ₃ H	1.078 B	C ₃ C ₄ H	127.9 B
C ₄ H	1.076 B	N ₁ C ₅ H	121.5 B
C ₅ H	1.077 B	N ₂ N ₁ H	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

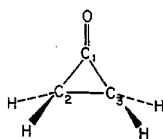
$\text{C}_3\text{H}_4\text{O}$

Bond	Substitution	Effective	Angle	Substitution	Effective
CO	1.219 C		CCO	123.3 C	
C ₁ C ₂	1.470 B		C ₂ C ₁ H	115.1 B	
C ₁ H	1.108 B		C ₁ C ₂ H	117.3 B	
C ₂ H	1.084 B		C ₁ C ₂ C ₃		119.8 C
C ₂ C ₃		1.345 B	C ₂ C ₃ H ₁		121.5 C
C ₃ H ₁		1.086 C	C ₂ C ₃ H ₂		120.0 C
C ₃ H ₂		1.086 C			

The C₃H₁ and C₃H₂ distances have been assumed to be equal.

[1] E. A. Cherniak and C. C. Costain, *J. Chem. Phys.* **45**, 104 (1966).

Cyclopropanone

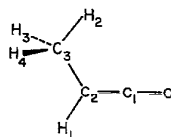
C₃H₄OC_{2v}

Bond	Substitution	Angle	Substitution
CO	1.191 E	C ₁ C ₂ C ₃	57.7 C
C ₁ C ₂	1.475 D	C ₂ C ₁ C ₃	64.6 C
C ₂ C ₃	1.575 D	HCH	114.1 D
CH	1.086 D	HC ₂ C ₁	118.5 D
		HC ₂ C 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

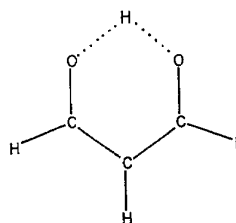
C₃H₄OC_s

Bond	Substitution	Effective	Angle	Substitution	Effective
C ₁ O	1.171 B		OC ₁ C ₂	179.5 C	
C ₁ C ₂	1.306 B		C ₁ C ₂ C ₃	122.6 B	
C ₂ C ₃	1.518 B		C ₁ C ₂ H ₁	123.7 B	
C ₂ H ₁	1.083 B		C ₂ C ₃ H ₂	111.1 B	
C ₃ H ₂	1.083 B		C ₂ C ₃ H ₃	110.7 ^a C	
C ₃ H ₃		1.094 ^a C	H ₃ C ₃ H 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).

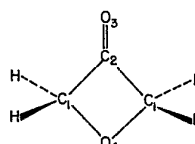
Malonaldehyde

C₃H₂O₂C_{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

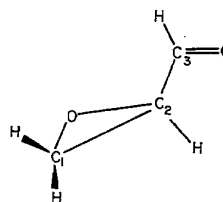
C₃H₄O₂C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
C ₁ C ₂	1.522 B		C ₁ C ₂ C ₁	88.1 B	
C ₁ O ₄ ^a		1.450 X	C ₂ C ₁ O ₄ ^a		88.5 X
C ₂ O ₃ ^a		1.230 X	C ₁ O ₄ C 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).

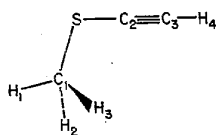
Oxiranecarboxaldehyde

C₃H₄O₂C₁

Bond	Substitution	Angle	Substitution
C ₁ C ₂	1.453 E	C ₁ C ₂ C ₃	119.8 D
C ₂ C 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

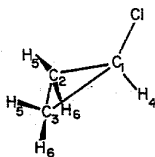
C₃H₄S C_s

Bond	Substitution	Effective	Angle	Substitution	Effective
SC ₁	1.813 B		C ₁ SC ₂		99.9 C
SC ₂		1.685 C	H ₁ C ₁ H ₂	110.0 B	
C ₂ C ₃		1.205 C	SC ₂ C ₃		178.0 C
C ₃ H ₄		1.061 C	H ₂ C ₁ H ₃	110.3 B	
C ₁ H ₁	1.079 B				
C ₁ H ₂	1.090 B				

The C₂C₃H₄ 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 Engelsens, J. Mol. Spectrosc. **30**, 474 (1969).

[2] D. den Engelsens, J. Mol. Spectrosc. **22**, 426 (1967).

Chlorocyclopropane
(Cyclopropyl chloride)C₃H₅Cl C_s

Bond	Substitution	Angle	Substitution
CCl	1.740 C	CCCl	118.7 C
C ₁ C ₂	1.513 C	ClCH	115.8 C
C ₂ C ₃	1.515 B	CCH ₄	116.1 C
CH ₄	1.079 B	C ₁ C ₃ H ₅	115.5 C
CH ₅	1.086 C	C ₁ C ₂ H ₆	117.8 C
CH ₆	1.082 C	C ₂ C ₃ H ₅	116.9 C
		C ₂ C ₃ H 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).

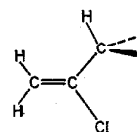
cis-1-ChloropropeneC₃H₃Cl CH₃-CH=CHCl C_s

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).

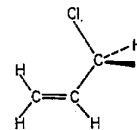
2-Chloropropene

C₃H₅Cl 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-ChloropropeneC₃H₅Cl C_s

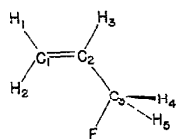
Rotational constants for two chlorine isotopic species were in agreement with a plane of symmetry. A second rotamer, with a dihedral angle of 122° about C—C bond, was also observed.

[1] E. Hirota, J. Mol. Spectrosc. **35**, 9 (1970).

Propanoyl Chloride
(Propionyl Chloride)C₃H₅ClO CH₃CH₂COCl 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.

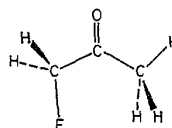
[1] H. Karlsson, J. Mol. Struct. **33**, 227 (1976).

cis-3-FluoropropeneC₃H₃FC_s

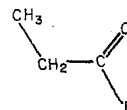
Bond	Substitution	Angle	Substitution
C ₁ C ₂	1.333 C	C ₁ C ₂ C ₃	124.6 C
C ₂ C ₃	1.488 C	C ₂ C ₃ F	111.7 C
C ₃ F	1.382 C	C ₂ C ₁ H ₁	120.9 C
C ₁ H ₁	1.080 C	C ₂ C ₁ H ₂	119.2 C
C ₁ H ₂	1.105 C	H ₁ C ₁ H ₂	119.9 C
C ₃ H ₄	1.098 C	C ₂ C ₃ H ₄	111.1 C
C ₃ H ₅	1.098 C	C ₂ C ₃ H ₅	111.1 C
		H ₄ C ₃ H ₅	108.1 C
		H ₄ C ₃ F	107.4 C
		H ₅ C ₃ F	107.4 C

C₂H₃ and C₁C₂H₃ parameters assumed.[1] E. Hirota, J. Chem. Phys. **42**, 2071 (1965).**gauche-3-Fluoropropene**C₃H₃FCH₂=CHCH₂FC₁

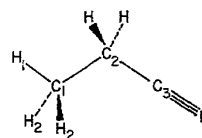
Bond	Substitution	Angle	Substitution
C ₁ C ₂	1.354 D	C ₁ C ₂ C ₃	121.6 D
C ₂ C ₃	1.486 D	C ₂ C ₃ F	110.9 D
C ₃ F	1.371 D	C ₂ C ₁ H ₁	119.2 D
C ₁ H ₁	1.098 D	C ₂ C ₁ H ₂	121.5 D
C ₁ H ₂	1.054 D	H ₁ C ₁ H ₂	119.3 D
C ₃ H ₄	1.127 D	C ₂ C ₃ H ₄	107.4 D
C ₃ H ₅	1.137 D	C ₂ C ₃ H ₅	105.2 D
		H ₄ C ₃ H ₅	111.4 D
		H ₄ C ₃ F	107.1 D
		H ₅ C ₃ F	114.7 D
		Dihedral*	127.1

Gauche form has CH₂F rotated 127.1 relative to *cis*. See *cis*-3-fluoropropene structure. C₂H₃ and C₁C₂H₃ parameters assumed.[1] E. Hirota, J. Chem. Phys. **42**, 2071 (1965).**1-Fluoro-2-propanone (Fluoroacetone)**C₃H₃FOC_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**C₃H₃FOC_s

Other than establishing this conformation as the most stable, no quantitative information was obtained about the structure.

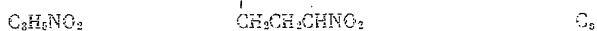
A *gauche* form, 1290 cal/mol less stable, was also observed. See the following.[1] O. Stiefvater and E. B. Wilson, J. Chem. Phys. **50**, 5385 (1969).**gauche-Propionyl Fluoride**C₃H₃FOCH₃CH₂COFC₁Dihedral angle between CCC and COF plane is 120° (E). A *cis* form, 1290 cal/mol more stable, was also observed. See the preceding.[1] O. Stiefvater and E. B. Wilson, J. Chem. Phys. **50**, 5385 (1969).**Propanenitrile
(Ethyl cyanide)**C₃H₃NC_s

Bond	Substitution	Angle	Substitution
C ₁ C ₂	1.537 B	C ₂ C ₃ N	178.7* D
C ₂ C ₃	1.459 C	C ₁ C ₂ C ₃	112.0 B
CN	1.159 C	C ₁ C ₂ H	110.6 B
C ₂ H	1.094 B	HC ₂ C ₃	108.1 B
C ₂ H ₁	1.079 D	HC ₂ H	107.2 B
C ₁ H ₂	1.091 B	H ₂ C ₁ H ₂	107.8 B
		H ₂ C ₁ C ₂	110.5 B
		H ₁ C ₁ C ₂	110.1 E

* The CN group is bent slightly toward the methyl group.

[1] H. M. Heise, H. Lutz and H. Dreizler, Z. Naturforsch. **29a**, 1345 (1974).

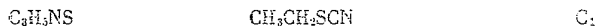
Nitrocyclopropane



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. Mochei, C. G. Britt, and J. E. Roggs, *J. Chem. Phys.* **56**, 3221 (1973).

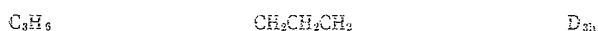
Ethyl Thiocyanate



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

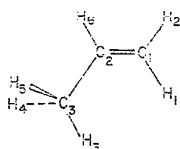


Bond	Effective	Angle	Effective
CH	1.083 C	HCH	114.0 C
CC	1.512 C		

In the calculation, $r_0(\text{C—H}) - r_0(\text{C—D}) = 0.002 \text{ \AA}$ 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).

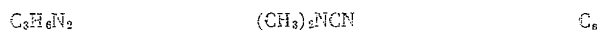
Propene (Propylene)



Bond	Substitution	Angle	Substitution
C_1C_2	1.336 B	$\text{H}_5\text{C}_3\text{H}_5$	106.2 D
C_2C_3	1.501 B	$\text{H}_1\text{C}_1\text{H}_2$	118.0 B
C_1H_1	1.091 B	$\text{H}_1\text{C}_1\text{C}_2$	120.5 B
C_1H_2	1.081 B	$\text{H}_2\text{C}_2\text{C}_1$	121.5 B
C_3H_5	1.090 B	$\text{C}_1\text{C}_2\text{C}_3$	124.3 B
C_3H_4	1.085 B	$\text{H}_2\text{C}_2\text{C}_3$	116.7 B
$\text{C}_3\text{H}_{4,5}$	1.098 D	$\text{H}_5\text{C}_3\text{C}_1$	119.0 B
		$\text{H}_5\text{C}_3\text{H}_2$	109.0 D
		$\text{H}_5\text{C}_3\text{C}_2$	111.2 B

- [1] D. R. Lide and D. Christensen, *J. Chem. Phys.* **35**, 1874 (1961).
 [2] E. Hirota and Y. Morino, *J. Chem. Phys.* **45**, 2325 (1966).

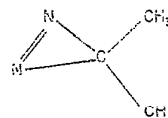
Dimethylcyanamide



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



Bond	Effective	Angle	Effective
CC	1.50 X	CCC	120 X
CN	1.49 X	H_aCH_a	109 X
NN	1.235 B	H_bCH_b	108 X
CH_a	1.08 X		
CH_b	1.10 X		

NCN and NNC angles assumed. H_a and H_b 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

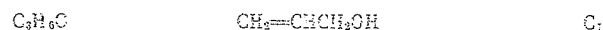


Bond	Substitution	Angle	Substitution
CC	1.507 B	CCC	117.2 B
CO	1.222 B	HCH	108.7 B
CH	1.085 C	2θ	119.9 B

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).

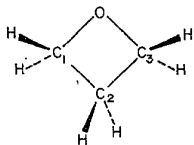
Allyl Alcohol



Molecule has *gauche* conformation. OH lies out of the plane and points toward the double bond.

- [1] A. N. Murty and R. P. Curl, Jr., *J. Chem. Phys.* **46**, 4176 (1967).

Oxetane
(Trimethylene Oxide)



C_3H_6O C_2v

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 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 C_1

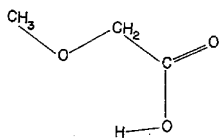


Angle	Effective
θ^a	131 X

^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



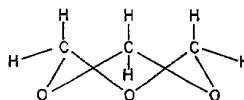
$C_3H_6O_3$ C_s

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).

J. Phys. Chem. Ref. Data, Vol. 8, No. 3, 1979

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 C_s

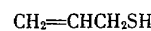


Cis conformation (with planar heavy atoms) was definitely established.

[1] R. E. Penn and R. F. Curl, Jr., J. Mol. Spectrosc. **24**, 235 (1967).

2-Propene-1-thiol (Allyl Mercaptan)

C_3H_6S C_1



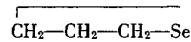
Angle	Effective
α	124 X
β	50 X

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 C_s



Angle	Effective
Dihedral	29.5 X

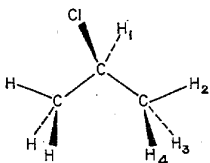
Various assumptions about vibrational motion required to obtain dihedral angle estimate.

[1] M. G. Petit, J. S. Gibson, and D. O. Harris, J. Chem. Phys. **53**, 3408 (1970).

2-Bromopropane

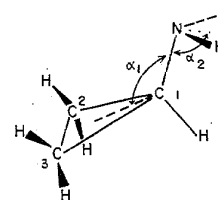
Bond	Substitution	Angle	Substitution
CBr	1.957 B	C CBr	110.0 B
CC	1.508 D	CCC	114.2 C

[1] R. H. Schwendeman and F. L. Tobiason, *J. Chem. Phys.* **43**, 201 (1965).

2-Chloropropane

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 ₃ CH ₄	109.1 C
		H ₂ CH ₃	109.1 C
		H ₂ CH ₄	108.7 C

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

**Cyclopropaneamine
(Cyclopropylamine)**

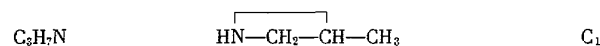
Bond	Substitution	Effective ^a	Angle	Substitution	Effective ^a
C ₁ C ₂	1.486 C		C ₂ C ₁ C ₃	61.2 B	
C ₂ C ₃	1.513 B		CCN		116.3 C
CN		1.462 D	CNH		111.0 E
NH		1.008 D	HNH		108.1 D
H...H	1.632 B		α ₁		121.0 C
			α ₂		127.5 X

^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).

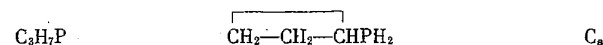
[2] M. D. Harmony, R. E. Bostrom and D. K. Hendricksen, *J. Chem. Phys.* **62**, 1599 (1975).

[3] M. D. Harmony, personal communication.

2-Methylaziridine (trans-Propyleneimine)

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_s conformation confirmed; see cyclopropylamine.

[1] L. A. Dinsmore, C. O. Britt, and J. E. Boggs, *J. Chem. Phys.* **54**, 915 (1971).

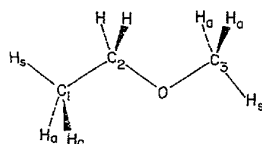
Propane.

C ₃ H ₈		CH ₃ CH ₂ CH ₃		C _{2v}	
Bond	Substitution	Angle	Substitution		
CC	1.526 B	CCC	112.4 B		
C ₂ H ₂ ^a	1.096 A	H ₂ CH ₂ '	106.1 A		
C ₁ H _b ^b	1.089 C	H _a CH _a	107.3 C		
C ₁ H _a	1.094 C	H _b CH _b	108.1 C		
		CCH _a	111.8 C		
		CCH _b	110.6 C		

^a C₂ is methylene carbon.

^b H_b 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 ₃ H ₈ O				C _s	
Bond	Substitution	Angle	Substitution		
C ₁ C ₂	1.520 B	C ₂ OC ₃	111.8 C		
C ₂ O	1.404 C	C ₁ C ₂ O	108.2 C		
C ₃ O	1.415 C	HC ₂ H	107.2 B		
C ₂ H	1.101 B	C ₁ C ₂ H	110.9 B		
C ₃ H _a	1.084 C	OC ₃ H _a	107.7 B		
C ₃ H _b	1.100 B	OC ₃ H _b	111.0 C		
C ₁ H _a	1.089 C	H _a C ₃ H _a	108.4 B		
C ₁ H _b	1.092 B	C ₂ C ₁ H _a	110.5 B		
		C ₂ C ₁ H _b	110.1 B		
		H _a C ₁ H _a	108.6 B		

[1] M. Hayashi and K. Kuwada, J. Mol. Struct. 28, 147 (1975).

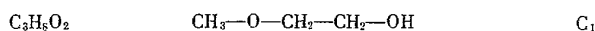
n-Propyl Alcohol

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).

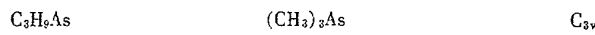
2-Methoxyethanol



Conformation has been shown to be *gauche* about each of the CH₃O-C, C-C and C-OH bonds.

[1] P. Buckley and M. Brochu, Can. J. Chem. 50, 1149 (1972).

Trimethylarsine

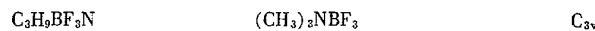


Bond	Effective
CAs	1.959 D

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).

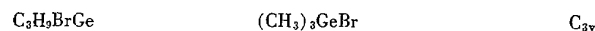
Trimethylamine-Boron Trifluoride



Bond	Substitution
BN	1.636 B

[1] P. S. Bryan and R. L. Kuczkowski, Inorg. Chem. 10, 200 (1971).

Bromotrimethylgermane

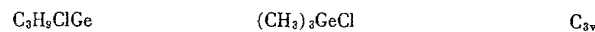


Bond	Substitution	Effective	Angle	Effective
GeBr	2.323 A		BrGeC ^a	106.3 C
GeC ^a		1.936 C		

^a Methyl group parameters were assumed to obtain this parameter.

[1] Y. S. Li and J. R. Durig, Inorg. Chem. 12, 306 (1973).

Trimethylchlorogermane



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).

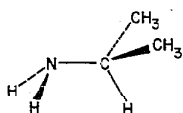
Chlorotrimethylsilane
(Trimethylchlorosilane)

C ₃ H ₉ ClSi		(CH ₃) ₃ SiCl		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



C₃H₉N 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 ₃ H ₉ N			(CH ₃) ₃ N			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 ₁ CH ₂		108.1 C	
			H ₂ CH ₃		108.6 C	

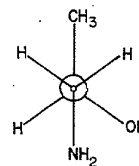
The H₂H₃ distance was assumed to be 1.7668 Å. The methyl groups are tilted 1.3° toward the nitrogen lone pair.

^a H₁ lies in plane of symmetry; H₂ and H₃ 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



C₃H₉NO C₁

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 ₃ H ₉ P		(CH ₃) ₃ P		C _{3v}
Bond	Substitution	Effective	Angle	Effective
CH ₃ ^a	1.112 D		PCH ₃	111.4 D
CH ₂ ^a		1.090 D	PCH ₂	109.8 D
PC		1.843 C	H ₃ CH ₃	108.2 D
			H ₃ CH ₂ ^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 ₃ H ₁₀ Ge		(CH ₃) ₃ GeH		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 ₃ H ₁₀ Si		(CH ₃) ₃ SiH		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 ₃ H ₁₂ BN		(CH ₃) ₃ NBH ₂		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 ₃ H ₁₂ BP			(CH ₃) ₃ PBH ₂			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 CH₃ 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 ₂ IN		I—C ¹ ≡C ² —C ³ ≡N		C _{∞v}
Bond		Substitution		
CI			1.985 B	
C ¹ C ²			1.207 B	
C ² C ³			1.370 A	
CN			1.160 A	

[1] T. Bjorvatten, *J. Mol. Struct.* **20**, 75 (1974).

C₄ Molecules

Butadiyne (Diacetylene)

C ₄ H ₂		HC ¹ ≡C ² —C ³ ≡C ⁴ H		D _{∞h}
Bond		Effective		
C ² C ³			1.376 X	
C ¹ H			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 ₄ H ₃ F ₃			F ₃ C ⁽¹⁾ —C ⁽²⁾ ≡C ⁽³⁾ —C ⁽⁴⁾ H ₂			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)

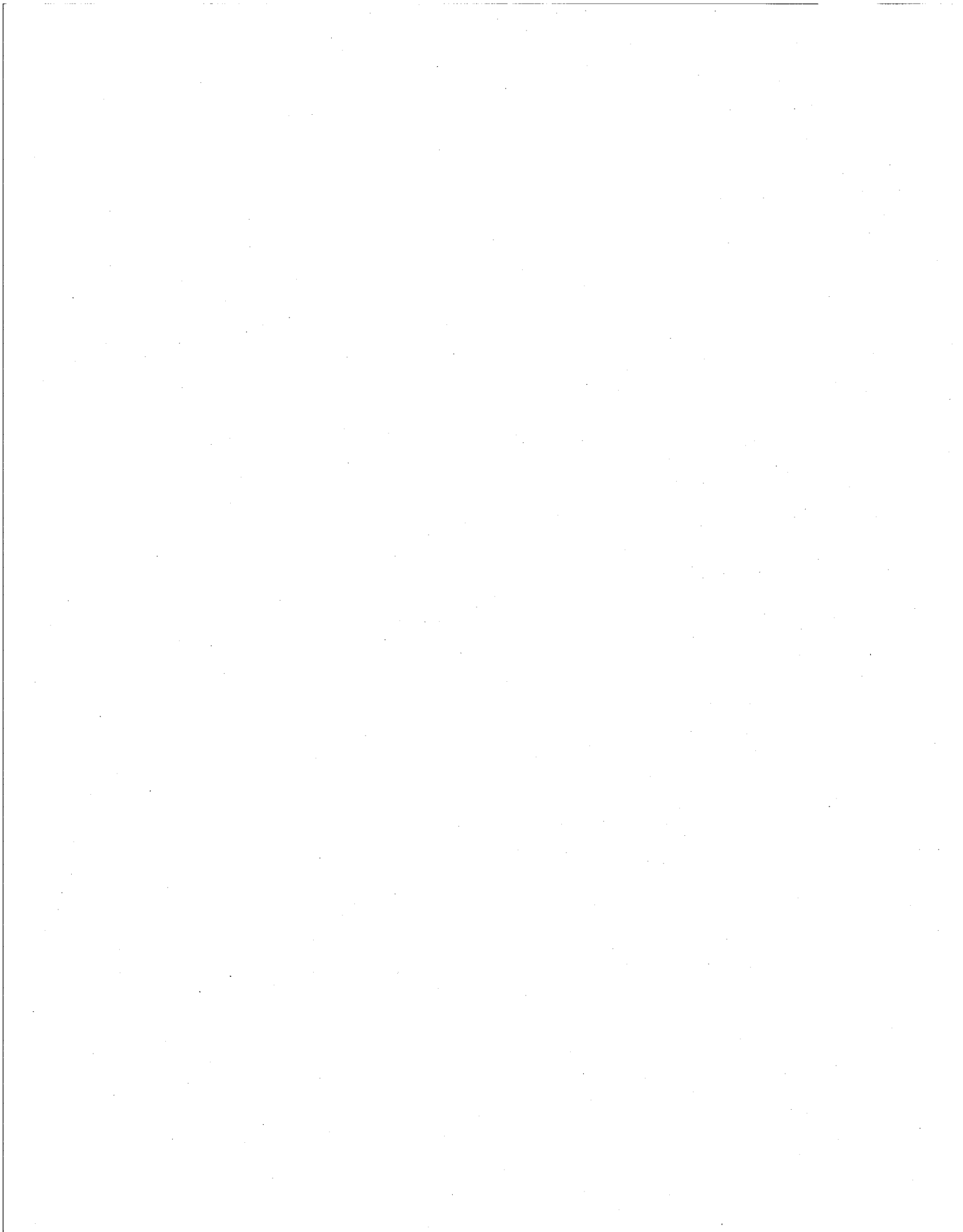
C ₄ H ₃ N		CH ₃ —C≡C—CN		C _{3v}
Molecular symmetry confirmed.				
[1] J. Sheridan and L. F. Thomas, <i>Nature</i> 174 , 798 (1954).				

Butatriene

C ₄ H ₄		C ¹ H ₂ =C ² =C ³ =C ⁴ H ₂		D _{2h}
Bond		Effective		
C ² C ³			1.284 X	

In order to derive the C²C³ bond distance it was necessary to assume HCH, C³C⁴, and C¹H. Because of the assumptions an estimate of the uncertainty in C²C³ can not be derived.

[1] B. P. Stoicheff, *Can. J. Phys.* **35**, 837 (1957).

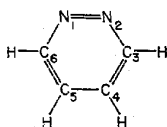


Trifluoroacetic Acid-Monofluoroacetic Acid Dimer

C ₄ H ₄ F ₄ O ₄		CF ₃ CO ₂ H · CFH ₂ CO ₂ H	
Bond		Effective	
O...O		2.69 X	

[1] C. G. Costain and G. P. Srivastava, *J. Chem. Phys.* **41**, 1620 (1964).

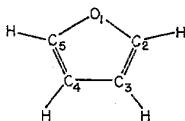
Pyridazine



C ₄ H ₄ N ₂			
Bond	Substitution	Angle	Substitution
NN	1.330 A	NNC	119.0 E
NC	1.353 E	NCC	123.7 E
C ₃ C ₄	1.382 E	CCC	117.3 E
C ₄ C ₆	1.375 A		

[1] W. Werner, H. Dreizler, and H. D. Rudolph, *Z. Naturforsch.* **22A**, 531 (1967).

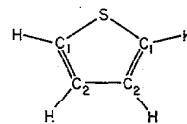
Furan



C ₄ H ₄ O			
Bond	Substitution	Angle	Substitution
CO	1.362 B	C ₅ OC ₂	106.5 B
C ₂ C ₃	1.361 B	OC ₂ C ₃	110.7 B
C ₃ C ₄	1.431 A	C ₂ C ₃ C ₄	106.0 B
C ₂ H	1.075 B	OC ₂ H	115.9 B
C ₃ H	1.077 A	C ₄ C ₃ H	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

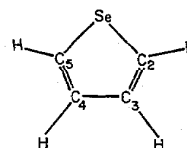


C ₄ H ₄ S			
Bond	Substitution	Angle	Substitution
SC	1.714 B	GSC	92.1 A
C ₁ C ₂	1.369 B	SC ₁ C ₂	111.5 A
C ₂ C ₃	1.423 B	C ₁ C ₂ C ₃	112.5 A
C ₁ H	1.078 B	SCH	119.8 B
C ₂ H	1.080 B	C ₂ C ₂ H	124.3 A

[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 ₄ H ₄ Se			
Bond	Substitution	Angle	Substitution
SeC ₂	1.855 A	C ₅ SeC ₂	87.8 B
C ₂ C ₃	1.369 B	SeC ₂ C ₃	111.6 B
C ₃ C ₄	1.433 B	C ₂ C ₃ C ₄	114.6 B
C ₂ H	1.070 B	SeC ₂ H ₂	121.7 B
C ₃ H	1.079 B	C ₄ C ₃ H 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 ₄ H ₃ Cl		ClH ₂ C—C≡C—CH ₃		C _s
Bond	Effective	Angle	Effective	
CH ^a	1.110°	HCH ^a	108.5°	
CH ^b	1.090°	HCH ^b	108.5°	
C≡C	1.207°	CCCl	111.5 X	
CC ^a	1.458 X			
CC ^b	1.460 X			
CCl	1.798 X			

^a Refers to CH₃ portion of molecule.

^b Refers to CH₂Cl 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 ₄ H ₅ ClO	(C ₃ H ₅)COCl	C _s
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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 ₄ H ₃ F ₃ O ₄		CF ₃ CO ₂ H·CH ₃ CO ₂ H	
Bond	Effective		
O···O	2.67 X		

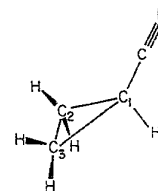
[1] C. C. Costain and G. P. Srivastava, J. Chem. Phys. **41**, 1620 (1964).

**Butenenitrile
(Allyl Cyanide)**

C ₄ H ₅ N	CH ₂ =CHCH ₂ CN
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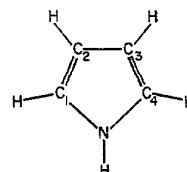
Two rotational isomers, "*cis*" and "*gauche*" were identified. No further structural analyses were performed.

[1] K. V. L. N. Sastry, V. M. Rao and S. C. Dass, Can. J. Physics **46**, 959 (1968).

**Cyclopropanecarbonitrile
(Cyclopropylcyanide)**

C ₄ H ₅ N		C _s	
Bond	Substitution	Angle	Substitution
C ₁ C ₂	1.528 C	C ₂ C ₁ C ₃	58.8 C
C ₂ C ₃	1.500 A	C ₁ C ₂ C ₃	60.6 C

[1] R. Pearson, Jr., A. Choplin and V. W. Laurie, J. Chem. Phys. **62** 4859 (1975).

Pyrrole

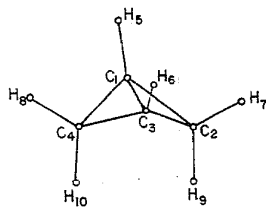
C ₄ H ₅ N		C _{2v}	
Bond	Substitution	Angle	Substitution
NC	1.370 B	CNC	109.8 B
C ₁ C ₂	1.382 B	NCC	107.7 B
C ₂ C ₃	1.417 B	CCC	107.4 B
NH	0.996 B	HC ₂ C ₃	127.1 B
C ₁ H	1.076 B	HC ₁ C ₂	130.7 B
C ₂ H	1.077 B		

[1] L. Nygaard, J. T. Nielsen, J. Kirchheiner, G. Maltesen, J. Rastrup-Andersen and G. O. Sørensen, 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

C₄H₆ C_{2v}

Bond	Substitution	Angle	Substitution
C ₂ C ₃	1.497 B	C ₁ C ₃ C ₂	60.0 A
C ₂ C ₃	1.498 B	C ₁ C ₂ C ₃	60.0 A
C ₂ H ₆	1.093 C	C ₂ C ₃ C ₄	98.3 B
C ₂ H ₇	1.093 C	HCH	115.6 B
C ₁ H ₅	1.071 B	H ₅ C ₂ C ₃	116.9 B
		H ₇ C ₂ C ₃	118.1 B
		C ₂ C ₃ H ₆	129.9 B
		C ₁ C ₃ H ₆	128.4 B

The dihedral angle between the heavy atom planes is 121.7°.

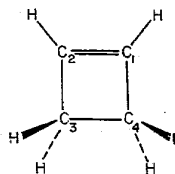
[1] K. W. Cox and M. D. Harmony, *J. Chem. Phys.* **50**, 1976 (1969).[2] M. D. Harmony and K. W. Cox, *J. Amer. Chem. Soc.* **88**, 5049 (1966).*trans*-1,3-ButadieneC₄H₆ C²H₂=C²HC²H=C²H₂ C_{2h}

Bond	Effective	Angle	Effective
C ² C ²	1.464 X	C ² C ² C ²	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).

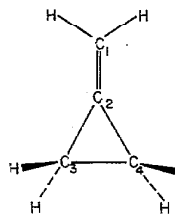
Cyclobutene

C₄H₆ C_{2v}

Bond	Substitution	Angle	Substitution
C ₁ C ₂	1.342 B	C ₁ C ₂ C ₃	94.2 B
C ₁ C ₄	1.517 B	C ₂ C ₃ C ₄	85.8 B
C ₂ C ₄	1.566 B	HC ₁ C ₂	133.5 B
C ₁ H	1.083 B	HC ₂ H	109.2 B
C ₃ H	1.094 B	HC ₃ C ₄	114.5 B
		α ^b	135.8 B

^a Angle between bisector of HCH and C₃C₄ bond.[1] B. Bak, J. J. Led, L. Nygaard, J. Rastrup-Andersen and G. O. Sorensen, *J. Mol. Struct.* **3**, 369 (1969).

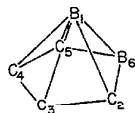
Methylenecyclopropane

C₄H₆ C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
C ₁ C ₂	1.332 B		C ₃ C ₂ C ₄	63.9 B	
C ₂ C ₃	1.457 B		HC ₁ H		114.3 D
C ₃ C ₄	1.542 A		HC ₃ H		113.5 D
C ₁ H		1.088 ^a	α ^b		29.2 D
C ₃ H		1.09 D			

Hydrogen parameters based upon assumed value of C₁H.^a Assumed value.^b Angle between HC₃H bisector and C₃C₄ bond axis.[1] V. W. Laurie and W. M. Stigliani, *J. Am. Chem. Soc.* **92**, 1485 (1970).

2,3,4,5-Tetracarbahexaborane (6)

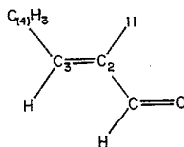
C₄H₆B₂C_s

Bond	Substitution
B ₁ B ₆	1.886 B
B ₁ C ₂	1.709 E
B ₁ C ₃	1.697 D
B ₆ C ₂	1.541 C
C ₂ C ₃	1.436 C
C ₃ C ₄	1.424 C

Above structure was that obtained by choosing the positive sign for small C₂ (and C₅) *c* coordinates. The other choice leads to a less reasonable B₁C₂ distance.

[1] J. P. Pasinski and R. A. Beaudet, *J. Chem. Phys.* **61**, 683 (1974).

trans-2-Butenal
(Crotonaldehyde)

C₄H₆OC_s

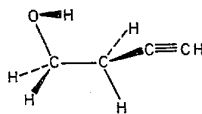
Angle ^a	Effective
C ₂ C ₃ C ₄	125.6 X
HC ₃ C ₄	116.1 X

^a Assumed values used for all other structural parameters.

[1] M. Suzuki and K. Kozima, *Bull. Chem. Soc. Japan* **42**, 2185 (1969).

[2] S. L. Hsu and W. H. Flygare, *Chem. Phys. Lett.* **4**, 317 (1969).

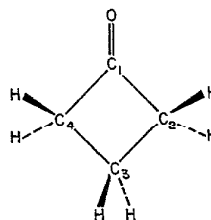
3-Butyn-1-ol

C₄H₆OC₁

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

C₄H₆OC_{2v}

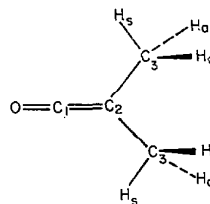
Bond	Substitution	Angle	Substitution
C ₁ C ₂	1.529 B	C ₂ C ₁ C ₄	93.0 B
C ₂ C ₃	1.556 B	C ₁ C ₂ C ₃	88.1 B
CO	1.204 C	C ₂ C ₃ C ₄	90.8 B
C ₂ H	1.099 B	HC ₂ H	109.2 C

The HC₂H 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

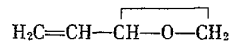
C₄H₆OC_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
CH _s	1.088 C		C ₁ C ₂ C ₃		120.6 X
CH _a	1.093 B		CCH _s		111.5 X
CO		1.171	CCH _a		110.6 X
C ₁ C ₂		1.300 X	H _a CH _a	107.3 C	
C ₂ C ₃		1.514 X	H _s CH _a	108.3 C	

CO bond length was fixed at value reported for ketene.

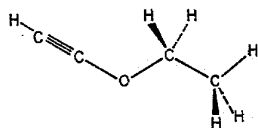
[1] K. P. R. Nair, H. D. Rudolph, and H. Dreizler, *J. Mol. Spectrosc.* **48**, 571 (1973).

3,4-Epoxy-1-butene

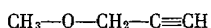
C₄H₆OC₁

The molecule was shown to exist in the *trans* conformation relative to the CC single bond.

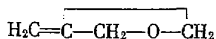
[1] T. Ikeda, K. V. L. N. Sastry and R. F. Curl, Jr., *J. Mol. Spectrosc.* **56**, 411 (1975).

EthoxyethyneC₄H₆OC_s

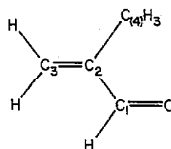
The spectrum of the *anti* conformation, shown above, is consistent with a planar heavy-atom skeleton. A less stable *gauche* form, having a dihedral angle about the CO bond of 108° (X), was also observed.

[1] A. Bjorseth, J. Mol. Struct. **20**, 61 (1974).**3-Methoxy-1-propyne
(Methylpropargyl ether)**C₄H₆OC₁

The observed stable molecular conformation was *gauche* with respect to the CO bond, the reported dihedral angle being 68° (0° = *syn* conformation).

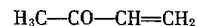
[1] K. M. Marstokk and H. Mollendal, J. Mol. Struct. **32**, 191 (1976).**3-Methyleneoxetane**C₄H₆OC_{2v}

Analysis of ground and excited states of the ring-puckering vibration indicated a planar heavy-atom equilibrium structure.

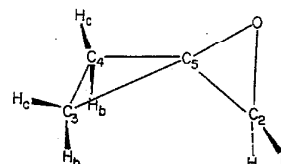
[1] J. S. Gibson and D. O. Harris, J. Chem. Phys. **52**, 5234 (1970).**trans-2-Methyl-2-propenal**C₄H₆OC_s

Angle ^a	Effective
C ₃ C ₂ C ₄	123.4 X
C ₁ C ₂ C ₃	116.4 X

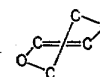
^a Assumed values used for all other structural parameters.

[1] M. Suzuki and K. Kozima, J. Mol. Spectrosc. **38**, 314 (1971).**Methyl vinyl ketone**C₄H₆OC_s

Observed conformation is that with the carbonyl *trans* to the vinyl group.

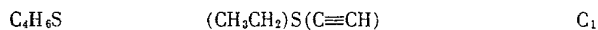
[1] P. D. Foster, V. M. Rao and R. F. Curl, Jr., J. Chem. Phys. **43**, 1064 (1965).**Oxaspiro[2.2]pentane**C₄H₆OC_s

Bond	Substitution	Angle	Substitution
C ₂ O	1.460 B	HC ₂ H	117.0 B
C ₃ C ₄	1.550 B	HC ₃ H	115.0 C
C ₃ C ₅	1.470 C	C ₂ O C ₅	60.4 B
C ₃ O	1.416 C	C ₂ C ₅ O	61.3 C
C ₂ C ₅	1.447 C	C ₃ C ₃ C ₄	63.6 C
C ₂ H	1.086 B	C ₃ C ₃ C ₄	58.2 C
C ₃ H _b	1.080 C	HC ₂ C ₅	119.5 B
C ₃ H _a	1.075 C	HC ₂ O	114.1 B
		H _b C ₃ H ₅	118.9 C
		H _b C ₃ C ₄	116.9 B
		H _c C ₃ C ₅	118.0 C
		H _c C ₃ C 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)**C₄H₄O₂C₂

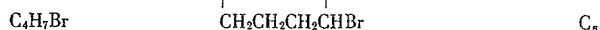
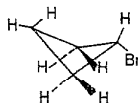
The twist (half-chair) conformation was reliably established.

[1] J. A. Wells and T. B. Malloy, Jr., J. Chem. Phys. **60**, 2132 (1974).

Ethylthioethyne

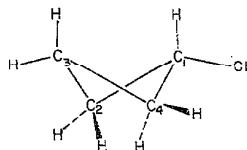
The observed spectrum was consistent only with the methyl group occupying a *gauche* conformation, 119° (X) from the *anti* position.

[1] A. Bjorseth, J. Mol. Struct. **23**, 1 (1974).

Bromocyclobutane

Ring is puckered with a dihedral angle of approximately 29°. Only the equatorial form was observed.

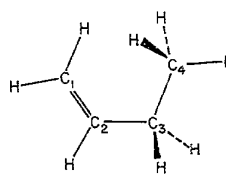
[1] W. G. Rothschild and B. P. Dailey, J. Chem. Phys. **36**, 2931 (1962).

Chlorocyclobutane

Bond	Effective	Angle	Effective
C ₁ Cl	1.775 D	HCCl	114 D
C ₁ C ₂	1.525 D	C ₂ C ₁ C ₄	91 D
C ₂ C ₃	1.550 D	HC ₂ H	112 D
C ₁ H	1.10 D	HC ₃ H	110 D
C ₂ H	1.09 D	HC ₂ C ₁	114 D
C ₃ H	1.10 D	ring dihedral	20 D
		CCl with C ₂ C ₁ C ₃ plane	135 D

CH₂ groups were assumed to bisect ring angles. Only equatorial Cl observed.

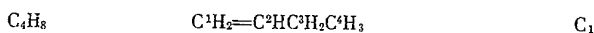
[1] H. Kim and W. D. Gwinn, J. Chem. Phys. **44**, 865 (1966).

cis-1-Butene

Bond	Effective	Angle	Effective
C ₁ C ₂	1.336 D	C ₁ C ₂ C ₃	126.7 D
C ₂ C ₃	1.507 D	C ₂ C ₃ C ₄	114.8 D
C ₃ C ₄	1.536 D	HC ₂ C ₃	115.1 D
		HC ₃ C ₃	110.4 D
		HC ₃ H	105.2 D

CH bond lengths were assumed. HC₃H was assumed to bisect C₂C₃C₄. The *skew* form was also observed. See the following.

[1] S. Kondo, E. Hirota, Y. Morino, J. Mol. Spectrosc. **28**, 471 (1968).

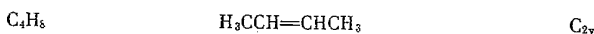
skew-1-Butene

Bond	Effective	Angle	Effective
C ¹ C ²	1.342 D	C ¹ C ² C ³	125.4 C
C ² C ³	1.493 D	C ² C ³ C ⁴	112.1 C
C ² C ⁴	1.536 D	dihedral ^a	119.9 C
		HC ² C ³	117.1 E
		HC ³ C ³	110.3 D
		HC ³ H	105.7 D

CH bond lengths were assumed. The *cis* form was also observed. See the preceding.

^a Angle between C¹C²C³ and C²C³C⁴ planes.

[1] S. Kondo, E. Hirota, and Y. Morino, J. Mol. Spectrosc. **28**, 471 (1968).

cis-2-Butene

Bond	Effective	Angle	Effective
CC	1.497 D	CCC	126.7 D

A number of structural parameters were assumed.

[1] S. Kondo, Y. Sakurai, E. Hirota, and Y. Morino, J. Mol. Spectrosc. **34**, 231 (1970).

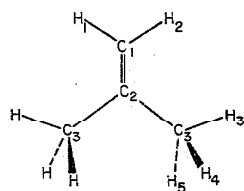


Cyclobutane

C ₄ H ₈ CH ₂ CH ₂ CH ₂ CH ₂ 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).

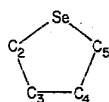
2-Methylpropene (isobutylene)



C ₄ H ₈ C _{2v}			
Bond	Substitution	Angle	Substitution
C ₁ C ₂	1.330 D	C ₁ C ₂ C ₃	115.3 D
C ₂ C ₃	1.507 C	H ₁ C ₁ H ₂	118.5 B
C ₂ H ₁	1.088 B	C ₂ C ₃ H ₅	112.9 E
C ₃ H ₃	1.072 E	C ₂ C ₃ H ₄	110.7 C
C ₃ H ₄	1.095 C	H ₁ C ₃ H 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 ₄ H ₈ Se C ₂			
Bond	Substitution	Angle	Substitution
SeC ₂	1.963 B	C ₂ SeC ₃	90.7 B
C ₂ C ₃	1.549 B	SeC ₂ C ₃	104.0 B
C ₃ C ₄	1.527 B	C ₂ C ₃ C ₄	106.9 C
		α ^a	29.7 C

^a Twist angle formed by intersection of C₂SeC₂ plane and C₄SeC₂ 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 ₄ H ₉ Cl (CH ₃) ₃ CCl 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 ₄ H ₉ F (CH ₃) ₃ CF 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 ₄ H ₉ GeN (CH ₃) ₃ GeCN 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 ₄ H ₉ I		(CH ₃) ₃ CI		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 ₄ H ₉ NOSi		(CH ₃) ₃ SiNCO		C _{3v}	
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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 ₄ H ₉ NSi		(CH ₃) ₃ SiCN		C _{3v}	
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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 ₄ H ₁₀		(CH ₃) ₂ CH		C _{3v}	
Bond	Substitution	Average	Angle	Substitution	Effective
CC	1.525 B	1.532 B	CCC		111.2 B
CH _t	1.108 B	1.109 B	CCH _a		109.4 C
CH _b	1.100 D	1.083 C	H _a CH _a ^a		108.5 D
CH _a	1.092 ^a D	1.083 C	H _a CH _b ^a		107.9 D

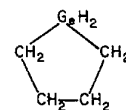
Average structure parameters are *r_z* values from combined microwave-electron diffraction data. H_t refers to tertiary hydrogen, and H_a and H_b refer to the in-plane and out-of-plane atoms, respectively.

^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

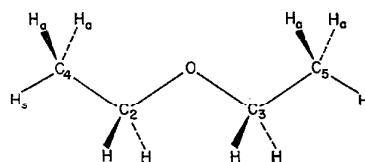


C ₄ H ₁₀ Ge		C ₂	
Angle ^a	Effective		
CGeC	98° X		
CCGe	106° X		
CCC	115° X		
Twist	18° X		

^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



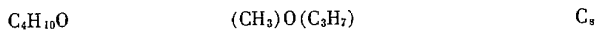
C ₄ H ₁₀ O		C _{2v}			
Bond	Substitution	Effective	Angle	Substitution	Effective
CO	1.408 B		COC		112.6 B
CC	1.516 B		OCC		108.6 B
C ₂ H	1.100 B		C ₄ C ₂ H		110.4 B
C ₄ H _a	1.090 B		OC ₂ H		109.9 B
C ₄ H _b	1.090 X		C ₂ C ₄ H _a		110.2 B
			C ₂ C ₄ H _b		110.6 D
			H _a C ₄ H _a		108.1 C
			H _b C ₄ H _b		108.6 C

The *b* coordinate of H_b was computed under the assumption that C₄H_a = C₄H_b. 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.

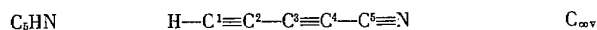
[2] M. Hayashi and K. Kuwada, *Bull. Chem. Soc. Japan* **44**, 299 (1971).

Methylpropyl ether



The observed spectrum is consistent only with the *trans-trans* conformation.

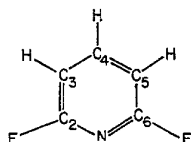
[1] M. Hayashi, M. Imachi, J. Nakagawa and A. Ozaki, Chem. Lett. (Japan) 1977, 41 (1977).

C_s-C₁₁ MoleculesCyanobutadiyne
(Cyanodiacetylene)

Bond	Substitution
CH	1.057 B
C ¹ C ²	1.209 A
C ² C ³	1.362 B
C ³ C ⁴	1.222 B
C ⁴ C ⁵	1.364 B
C ⁵ N	1.161 A

[1] A. J. Alexander, H. W. Kroto and D. R. M. Walter, J. Mol. Spectrosc. 62, 175 (1976).

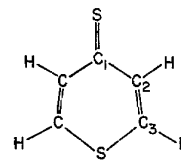
2,6-Difluoropyridine



Bond	Substitution	Effective	Angle	Substitution	Effective
NC ₂	1.317 B		C ₃ C ₄ C ₅	119.8 A	
C ₂ C ₃	1.377 C		C ₂ C ₃ C ₄	116.1 A	
C ₃ C ₄	1.394 A		NC ₂ C ₃	126.5 B	
C ₃ H	1.080 B		C ₂ NC ₆	115.0 B	
C ₄ H	1.082 B		C ₃ C ₄ H	120.1 B	
C ₂ F		1.347 B	C ₂ C ₃ H	120.8 B	
			C ₃ C ₂ F		118.8 B

[1] O. L. Stiefvater, Z. Naturforsch. 30a, 1765 (1975).

4H-Thiapyran-4-thione

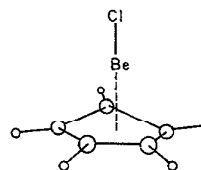


Bond	Substitution	Angle	Substitution
C ₁ S	1.671 B	C ₂ C ₁ C ₂	117.5 D
C ₃ S	1.759 A	C ₁ C ₂ C ₃	128.1 D
C ₁ C ₂	1.406 ^a D	C ₂ C ₃ S	122.4 C
C ₂ C ₃	1.342 ^a D	C ₃ SC ₂	101.4 A

^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



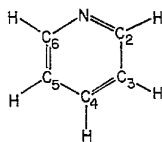
Bond	Substitution	Effective
CC	1.424 B	1.424 B
BeCl	1.81 E	1.839 C
h ^a	1.52 E	1.485 C
CH	1.09 E	1.090 D
Cl...C	3.546 B	3.538 B

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

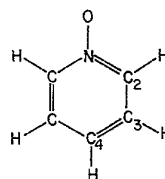


C ₅ H ₅ N		C _{2v}	
Bond	Substitution	Angle	Substitution
NC ₂	1.338 A	C ₅ NC ₂	116.9 A
C ₂ C ₃	1.394 B	NC ₂ C ₃	123.8 A
C ₃ C ₄	1.392 A	C ₂ C ₃ C ₄	118.5 A
C ₂ H	1.086 B	C ₃ C ₄ C ₅	118.4 A
C ₃ H	1.082 B	NC ₂ H	116.0 B
C ₄ H	1.081 B	C ₂ C ₃ H	120.1 B
		C ₃ C ₄ H	120.8 B

[1] G. O. Sorensen, L. Moller 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).

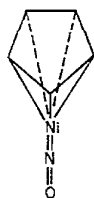
Pyridine N-oxide



C ₅ H ₅ NO			C _{2v}	
Bond	Substitution	Effective	Angle	Substitution
NC ₂	1.362 C		CNC	119.8 C
C ₂ C ₃	1.389 C		NCC	120.7 B
C ₃ C ₄	1.395 A		C ₂ C ₃ C ₄	120.6 A
NO		1.278 D	C ₃ C ₄ C ₅	117.6 A

Hydrogen parameters were assumed to obtain the NO distance.

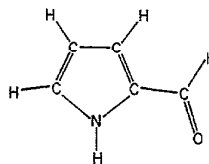
[1] O. Snerling, C. J. Nielsen, L. Nygaard, E. J. Pedersen and G. O. Sorensen, *J. Mol. Struct.* **27**, 205 (1975).

 π -Cyclopentadienylnitrosylnickel

C ₅ H ₅ NNiO			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 C₅H₅ ring system (i.e., coplanarity of C₅, H₅ planes) was obtained. The CH distances were assumed.

[1] A. P. Cox and A. H. Brittain, *Trans. Faraday Soc.* **66**, 557 (1970).

cis-Pyrrole-2-carboxaldehyde

C ₅ H ₅ NO		C _s
The <i>cis</i> 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).

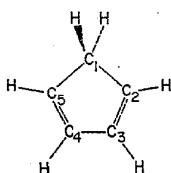
Cyclopentadienyl Thallium

C ₅ H ₅ Tl		C _{5v}
Bond	Effective	
CC	1.43 X	
CTl	2.705 X	

C₅H₅ 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).

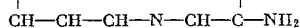
Cyclopentadiene

C₅H₆ C_{2v}

Bond	Substitution	Angle	Substitution
C ₁ C ₂	1.506 B	C ₂ C ₁ C ₂	102.9 B
C ₂ C ₃	1.344 B	C ₁ C ₂ C ₃	109.2 B
C ₃ C ₄	1.468 B	C ₂ C ₃ C ₄	109.3 B
C ₁ H	1.099 B	HC ₁ H	106.3 B
C ₂ H	1.078 B	HC ₂ C ₃	127.1 B
C ₃ H	1.080 B	HC ₃ C ₂	126.0 B

[1] D. Damiani, L. Ferretti and E. Gallinella, Chem. Phys. Lett. 37, 265 (1976).

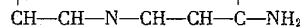
[2] L. H. Scharpen and V. W. Laurie, J. Chem. Phys. 43, 2765 (1965).

3-Pyridinamine
(3-Aminopyridine)C₅H₆N₂ C₁

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 $d(\text{NH}) = 1.00$ 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.

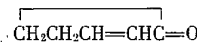
4-Pyridinamine
(4-Aminopyridine)C₅H₆N₂ C_s

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 $d(\text{NH}) = 1.00$ 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.

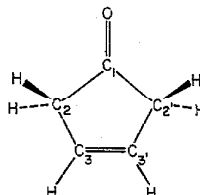
Cyclopent-2-en-1-one

C₅H₆O 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

C₅H₆O C_{2v}

Bond	Substitution	Angle	Substitution
CO	1.210 A	C ₂ C ₁ C _{2'}	109.2 C
C ₁ C ₂	1.524 C	C ₁ C ₂ C ₃	103.1 C
C ₂ C ₃	1.509 C	C ₂ C ₃ C _{3'}	112.4 B
C ₃ C _{3'}	1.338 B	HC ₂ H	107.3 C
C ₂ H	1.086 B	HC ₃ C ₂	124.7 B
C ₃ H	1.079 B	θ ^a	0.0 C

^a Angle between the bisectors of the HC₂H and C₁C₂C₃ angles.

[1] J. W. Bevan and A. C. Legon, J. Chem. Soc. Faraday Trans., 67, 902 (1973).

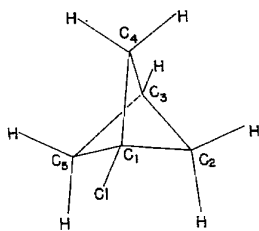
2-Methylfuran

C₅H₆O 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

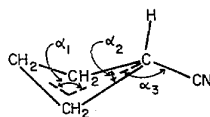
C₅H₇Cl C_{3v}

Bond	Effective	Angle	Effective
C ₁ C ₂	1.536 X	C ₁ C ₂ C ₃	73.5 X
C ₂ C ₃	1.556 X	C ₂ C ₁ C ₄	88.6 X
C ₁ Cl	1.761 X	C ₂ C ₃ C ₄	87.2 X
		ClC ₁ C ₂	126.2 X

In order to obtain the structural parameters, the constraint $r(C_2C_3) - r(C_1C_2) = 0.02 \pm 0.01 \text{ \AA}$ 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

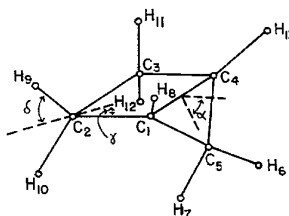
C₄H₇N C_s

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

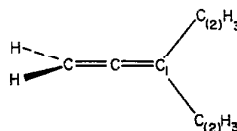
C₅H₈ C_s

Bond	Substitution	Angle	Substitution
C ₁ C ₄	1.536 B	C ₁ C ₂ H ₉	113.3 D
C ₂ C ₃	1.565 B	C ₁ C ₂ H ₁₀	115.2 C
C ₁ C ₂	1.528 C	C ₃ C ₂ H ₉	111.9 C
C ₁ C ₅	1.507 B	C ₃ C ₂ H ₁₀	116.6 D
C ₅ H ₆	1.088 B	H ₆ C ₅ H ₇	116.7 C
C ₅ H ₇	1.090 B	H ₆ C ₁ C ₅	121.2 C
C ₁ H ₈	1.082 B	H ₆ C ₁ C ₄	128.6 C
C ₂ H ₉	1.085 C	α	67.3 C
C ₂ H ₁₀	1.097 C	β	61.0 C

Redundant parameters: H₆C₅C₁ = 114.7 (C), H₇C₅C₁ = 119.0 (B), H₈C₁C₂ = 126.3 (C), H₉C₂H₁₀ = 109.4 (C), γ = 44.8 (C), δ = 57.3 (D). Angle β is the acute angle formed by the intersection of C₅H₆ with the bisector of the C₁C₄C₅ angle.

[1] S. N. Mathur, M. D. Harmony and R. D. Suenram, *J. Chem. Phys.* **64**, 4340 (1976).

Dimethylallene

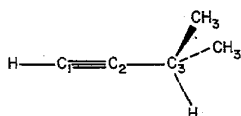
C₃H₄ C_{2v}

Bond	Effective	Angle	Effective
C ₁ C ₍₂₎	1.514 X	C ₍₂₎ C ₁ C ₍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

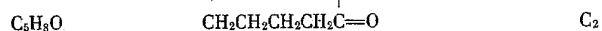


C ₅ H ₈		C _s	
Bond	Effective	Angle	Effective
C _{M_e} C ₃	1.527 X	C _{M_e} C ₃ C ₂	109.6 X
C ₂ C ₃	1.495 X	C _{M_e} CC _{M_e}	112.9 X
C ₁ C ₂ ^a	1.203 A	HC ₁ C ₂ ^a	180.0
C ₁ H ^a	1.058 A	HC _{M_e} H ^a	109.5
C _{M_e} H ^a	1.092		

^a Assumed value.

[1] A. R. Mochel, A. Bjørseth, C. O. Britt, and J. E. Boggs, *J. Mol. Spectrosc.* **48**, 107 (1973).

Cyclopentanone



The ground state conformation is a twisted C₂ form.

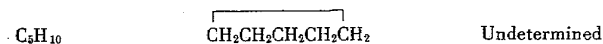
[1] H. Kim and W. D. Gwinn, *J. Chem. Phys.* **51**, 1815 (1969).

Pivalonitrile
(Tertiary Butyl Cyanide)

C ₅ H ₉ N		(C ¹ H ₃) ₃ C ² C ³ N		C _{3v}
Bond	Substitution	Angle	Substitution	
C ³ N	1.159 A	C ¹ C ² C ¹	110.5 C	
C ¹ C ²	1.536 C			
C ² C ³	1.478 C			

[1] L. J. Nugent, D. E. Mann and D. R. Lide, *J. Chem. Phys.* **36**, 965 (1962).

Cyclopentane



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 ₆ H ₃ F ₃		D _{3h}
Bond	Effective	
CF	1.304 X	

In order to determine r₀(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 ₆ H ₄ ClF		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 ₆ H ₄ ClF		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 ₆ H ₄ F 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)

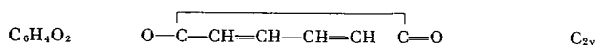
Bond	Effective
CC	1.40 X
CH	1.084 X
CF	1.31 X

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



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).

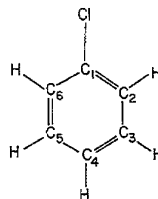
Bromobenzene

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

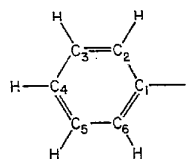


Bond	Substitution		Angle	Substitution	
	Effective	Effective		Effective	Effective
C_1C_2	1.399 B	1.402 B	$C_6C_1C_2$	120.2 B	120.2 B
C_2C_3	1.386 C	1.390 C	$C_1C_2C_3$	119.8 B	119.7 B
C_3C_4	1.398 A	1.398 A	$C_2C_3C_4$	120.2 A	120.2 A
C_1Cl	1.725 B	1.722 B	$C_3C_4C_5$	119.8 A	120.0 A
C_3H	1.080 C	1.077 C	ClC_1C_2	119.9 B	119.9 B
C_2H	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



Bond	Substitution		Angle	Substitution	
	Effective	Effective		Effective	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_5H	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 I. Rastrup-Andersen, *J. Mol. Struct.* **2**, 209 (1968).

Iodobenzene

C ₆ H ₅ I		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).

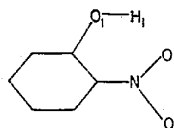
Nitrosobenzene

C ₆ H ₅ NO				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



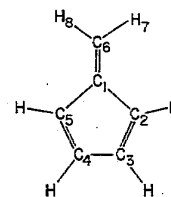
C ₆ H ₅ NO ₂		C _s
Bond	Substitution	
O ₁ H ₁	1.00 D	

[1] S. Leavell and R. F. Curl, Jr., *J. Mol. Spectrosc.* **45**, 428 (1973).

Benzene

C ₆ H ₆		D _{6h}
Bond	Effective	
CC	1.396 B	
CH	1.083 B	

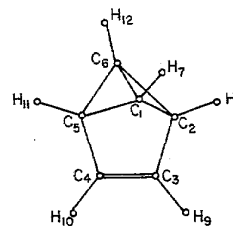
[1] A. Cabana, J. Bachand and J. Giguere, *Can. J. Phys.* **52**, 1949 (1974).

5-Methylene-1,3-Cyclopentadiene
(Fulvene)

C ₆ H ₆				C _{2v}
Bond	Substitution	Angle	Substitution	
C ₁ C ₆	1.348 A	C ₂ C ₁ C ₅	106.8 A	
C ₁ C ₂	1.468 A	C ₁ C ₂ C ₃	107.7 A	
C ₂ C ₃	1.357 A	C ₂ C ₃ C ₄	108.9 A	
C ₃ C ₄	1.476 A	C ₁ C ₂ H	124.9 A	
C ₄ H	1.077 A	C ₂ C ₃ H	126.4 A	
C ₅ H	1.080 A	H ₇ C ₆ H ₈	118.1 A	
C ₆ H 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).

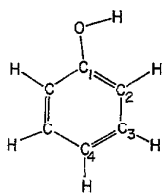
Tricyclo[3.1.0.0^{2,6}]hex-3-ene
(Benzvalene)

C ₆ H ₆				C _{2v}
Bond	Substitution	Angle	Substitution	
C ₁ C ₆	1.452 A	α ^a	106.0 C	
C ₁ C ₂	1.529 B	C ₆ C ₁ H ₇	133.7 A	
C ₂ C ₃	1.503 C	C ₂ C ₁ H ₇	135.3 A	
C ₃ C ₄	1.339 A	C ₁ C ₂ H ₈	119.8 C	
C ₁ H ₇	1.078 A	C ₃ C ₂ H ₃	124.2 C	
C ₂ H ₈	1.082 A	C ₂ C ₃ H ₉	125.4 A	
C ₃ H ₉	1.078 A	C ₁ C ₂ H ₈	128.9 A	
		C ₃ C ₂ C 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

C₆H₅O C_s

Bond	Effective	Substitution	Angle	Effective
CC	1.397 X		COH	109.0 X
C ₂ H	1.084 X		OC ₁ C ₂	122.2 X
C ₃ H	1.076 X			
C ₄ H	1.082 X			
CO	1.364 X			
OH		0.956 X		

Assumed:

Ring is a regular hexagon.

C₂ 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).

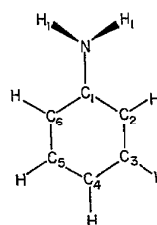
Thiophenol

C₆H₅S C_sC₆H₅SH

Data are consistent with planarity.

[1] K. I. Johansson, H. Oldeberg and H. Selen, Arkiv. Fysik. **33**, 313 (1967).

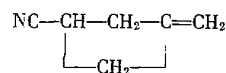
Aniline

C₆H₇N C_s

Bond	Substitution	Angle	Substitution
NH ₁	1.001 D	H ₁ NH ₁	113.1 D
C ₁ N	1.402 B	C ₆ C ₁ C ₂	119.4 A
C ₁ C ₂	1.397 B	C ₁ C ₂ C ₃	120.1 A
C ₂ C ₃	1.394 B	HC ₂ C ₃	120.1 A
C ₃ C ₄	1.396 B	C ₂ C ₃ C ₄	120.7 A
C ₂ H	1.082 B	HC ₃ C ₂	119.4 A
C ₃ H	1.083 B	C ₃ C ₄ C ₅	118.9 A
C ₄ H	1.080 B		

The C₆H₅N fragment is essentially planar. The dihedral angle between the NH₂ and C₆H₅N 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).

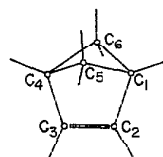
3-Methylenecyclobutanecarbonitrile

C₆H₇N C_s

The ring is non-planar with the CN group in the equatorial position.

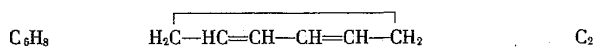
[1] J. R. Durig, Y. S. Li, M. D. Harmony and M. Y. Fong, J. Mol. Struct. **23**, 377 (1974).

Bicyclo[2.1.1]hex-2-ene

C₆H₈ C_{2v}

Bond	Substitution	Angle	Substitution
C ₁ C ₂	1.528 B	C ₁ C ₂ C ₃	103.3 C
C ₂ C ₃	1.341 B	C ₅ C ₁ C ₂	100.4 C
C ₁ C ₅	1.568 B	C ₅ C ₁ C ₆	85.3 C
		C ₁ C ₅ C ₄	81.4 C
		θ ^a	126.7 C

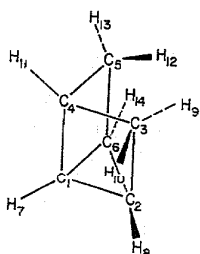
^a Dihedral angle formed by intersection of C₄C₅C₁ and C₄C₆C₁ planes.[1] C. S. Wang and M. D. Harmony, J. Am. Chem. Soc. **98**, 1976.

1,3-Cyclohexadiene

Angle	Effective
τ	17.5 X

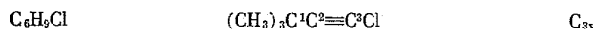
τ is the torsional angle between the two double bonds.

[1] S. S. Butcher, J. Chem. Phys. **42**, 1830 (1965).

Tricyclo[2.2.0.0^{2,6}]hexane

Bond	Substitution	Effective	Angle	Substitution	Effective
C ₁ C ₂	1.513 B	1.518 C	H ₃ C ₃ H ₁₀	110.2 C	110.7 C
C ₁ C ₄	1.584 B	1.589 C	C ₁ C ₄ H ₁₁	126.4 B	126.5 B
C ₂ C ₃	1.523 B	1.527 B	C ₂ C ₄ H ₁₁	120.9 B	120.9 B
C ₂ C ₆	1.533 B	1.541 C	C ₄ C ₁ H ₇	134.6 B	134.5 B
C ₃ C ₄	1.549 B	1.553 B	C ₂ C ₁ H ₇	131.9 B	131.8 B
C ₁ H ₇	1.079 C	1.077 C	C ₁ C ₂ H ₈	127.4 B	127.4 B
C ₂ H ₈	1.082 C	1.080 C	C ₃ C ₂ H ₈	120.6 B	120.5 B
C ₃ H ₉	1.099 C	1.098 C	C ₂ C ₃ H ₈	128.4 B	128.6 B
C ₃ H ₁₀	1.087 C	1.090 C	C ₁ C ₂ C ₃	91.8 B	
C ₄ H ₁₁	1.086 C	1.086 C	C ₂ C ₃ C ₄	86.2 A	
			C ₃ C ₄ C ₁	88.2 A	
			C ₄ C ₁ C ₂	85.4 A	
			C ₁ C ₂ C ₆	59.6 A	
			C ₂ C ₁ C 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)**

Bond	Substitution	Effective
C ³ Cl	1.638 B	
C ¹ ...C ³	2.671 B	
C ¹ C ² *	1.47 X	1.47 D

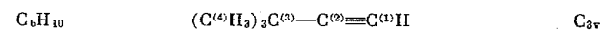
* $r(\text{C}^1\text{C}^2)$ calculated assuming $r(\text{C}^2\text{C}^3)$ is 1.205 Å.

[1] H. Bodensch, R. Gegenheimer, J. Mennicke and W. Zeil, Z. Naturforsch. **22A**, 523 (1967).

Cyclohexene

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)**

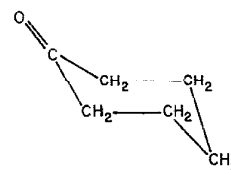
Bond	Substitution	Angle	Substitution
C ⁽¹⁾ H	1.056 A	C ⁽²⁾ C ⁽³⁾ C ⁽⁴⁾	108.0 C
C ⁽¹⁾ C ⁽²⁾	1.209 A		
C ⁽²⁾ C ⁽³⁾	1.496 D		
C ⁽³⁾ C ⁽⁴⁾	1.532 C		

[1] L. J. Nugent, D. E. Mann and D. R. Lide, Jr., J. Chem. Phys. **36**, 965 (1962).

1,1-Difluorocyclohexane

The microwave data show that the molecule adopts the chair conformation.

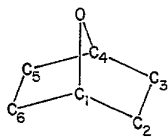
[1] D. Damiani and L. Ferretti, Chem. Phys. Lett. **24**, 357 (1974).

Cyclohexanone

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

C₆H₁₀OC_{2v}

Bond	Substitution	Effective	Angle	Substitution
C ₁ C ₂	1.537 B		C ₁ C ₂ C ₃	101.2 B
C ₂ C ₃	1.551 B		C ₂ C ₁ C ₆	109.9 B
C ₁ O		1.452 C		

Hydrogen parameters were assumed to obtain the CO distance.

[1] R. A. Creswell, *J. Mol. Spectrosc.* **56**, 133 (1975).

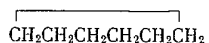
Fluorocyclohexane

C₆H₁₁FC_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

C₆H₁₂D_{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

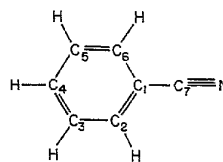
C₆F₆D_{6h}

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

C₇H₅NC_{2v}

Bond	Substitution	Angle	Substitution
C ₁ C ₂	1.388 C	C ₆ C ₁ C ₂	121.8 C
C ₂ C ₃	1.396 C	C ₁ C ₂ C ₃	119.0 B
C ₃ C ₄	1.397 B	C ₂ C ₃ C ₄	120.1 A
C ₁ C ₇	1.451 B	C ₃ C ₄ C ₃	120.1 A
C ₇ N	1.158 A	C ₃ C ₃ H	120.4 C
C ₂ H	1.080 C	C ₂ C ₃ H	120.0 A
C ₃ H	1.082 B		
C ₄ H	1.080 A		

[1] J. Casado, L. Nygaard, and G. O. Sørensen, *J. Mol. Struct.* **8**, 211 (1971).

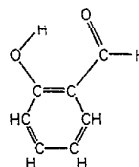
[2] B. Bak, D. Christensen, W. B. Dixon, L. Hansen-Nygaard, and J. Rastrup-Andersen, *J. Chem. Phys.* **37**, 2027 (1962).

Isocyanatobenzene
(Phenylisocyanate)C₇H₅NOC₆H₅NCOC₂

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).

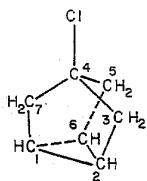
Salicylaldehyde

C₇H₆O₂C_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^{2,5}]heptane
(4-Chloronortricyclene)

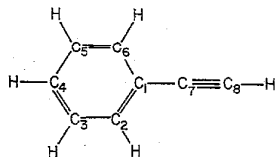
C₇H₆ClC_{2v}

Bond	Substitution	Angle	Substitution
C ₄ Cl	1.763 ^a	ClC ₄ C ₇	115.7 D
C ₇ C ₄	1.538 D	C ₇ C ₄ C ₃	102.6 B
C ₁ C ₇	1.525 D	C ₁ C ₇ C ₄	96.2 C
C ₁ C ₂	1.527 B	C ₂ C ₁ C ₇	106.6 C

^aThis distance was assumed with an uncertainty of ± 0.003 Å in order to determine the C₄ substitution coordinate.

[1] V. W. Laurie and W. M. Stigliani, J. Am. Chem. Soc. 95, 4154 (1973).

Ethynyl benzene
(Phenyl acetylene)

C₈H₆C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
C ₁ C ₅		1.388 C	C ₅ C ₁ C ₆		120.8 C
C ₂ C ₃		1.396 D	C ₁ C ₂ C ₃		119.8 B
C ₃ C ₄	1.398 A		C ₂ C ₃ C ₄		119.9 B
C ₁ C ₇		1.448 C	C ₃ C ₄ C ₅	119.9 A	
C ₇ C ₈	1.208 A				
C ₈ H	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).

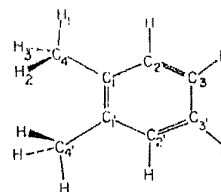
7-Methylene-1,3,5-cycloheptatriene
(Heptatfulvene)

C₈H₆C_{2v}

The observed microwave spectrum confirmed the planar conformation.

[1] A. Bauder, C. Keller and M. Neuenschwander, J. Mol. Spectrosc. 63, 231 (1976).

ortho-Xylene

C₈H₁₀C_{2v}

Bond	Substitution	Effective	Angle	Substitution	Effective
C ₄ H ₁	1.080 B		H ₁ C ₄ H ₂		108.9 C
C ₄ H ₂	1.095 B		H ₂ C ₄ H ₃		106.0 D
C ₁ C ₄		1.509 X	C ₄ C ₁ C ₂		121.1 X
C ₁ C ₂		1.414 X	C ₂ C ₁ C _{1'}		119.8 X
C ₁ C _{1'}		1.394 X	C ₁ C ₂ H		118.9 X
C ₂ H		1.072 X	C ₂ C ₃ H		119.7 X
C ₃ H		1.079 X	H ₁ C ₄ C ₁		111.2 X
			H ₂ C ₄ C ₁		111.0 X

[1] H. D. Rudolph, K. Walzer and I. Krutzik, J. Mol. Spectrosc. 47, 314 (1973).

1-Cyanoadamantane

C₁₁H₁₆NC₁₀H₁₀CNC_{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).