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Selected Values of Electric Dipole Moments for Molecules in the Gas Phase

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Foreword

The National Standard Reference Data System is a government-wide effort to give to the technical community of the United States optimum access to the quantitative data of physical science, critically evaluated and compiled for convenience. This program was established in 1963 by the President's Office of Science and Technology, acting upon the recommendation of the Federal Council for Science and Technology. The National Bureau of Standards has been assigned responsibility for administering the effort. The general objective of the System is to coordinate and integrate existing data evaluation and compilation activities into a systematic, comprehensive program, supplementing and expanding technical coverage when necessary, establishing and maintaining standards for the output of the participating groups, and providing mechanisms for the dissemination of the output as required.

The NSRDS is conducted as a decentralized operation of nation-wide scope with central coordination by NBS. It comprises a complex of data centers and other activities, carried on in government agencies, academic institutions, and nongovernmental laboratories. The independent operational status of existing critical data projects is maintained and encouraged. Data centers that are components of the NSRDS produce compilations of critically evaluated data, critical reviews of the state of quantitative knowledge in specialized areas, and computations of useful functions derived from standard reference data.

For operational purposes, NSRDS compilation activities are organized into seven categories as listed below. The data publications of the NSRDS, which may consist of monographs, loose-leaf sheets, computer tapes, or any other useful product, will be classified as belonging to one or another of these categories. An additional "General" category of NSRDS publications will include reports on detailed classification schemes, lists of compilations considered to be Standard Reference Data, status reports, and similar material. Thus, NSRDS publications will appear in the following eight categories:

<i>Category</i>	<i>Title</i>
1	General
2	Nuclear Properties
3	Atomic and Molecular Properties
4	Solid State Properties
5	Thermodynamic and Transport Properties
6	Chemical Kinetics
7	Colloid and Surface Properties
8	Mechanical Properties of Materials

The present compilation is in category 3 of the above list. It constitutes the tenth publication in the new NBS series known as the National Standard Reference Data Series.

A. V. ASTIN, *Director.*

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Selected Values of Electric Dipole Moments for Molecules in the Gas Phase

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This table revises, brings up to date, and extends the coverage on numerical values for dipole moments which was included in NBS Circular 537, Tables of Dielectric Constants and Electric Dipole Moments of Substances in the Gaseous State, prepared by Maryott and Buckley in 1953. A recommended value with an estimate of accuracy is presented for more than five hundred organic and inorganic compounds. Extensive comments are given on the definition of dipole moment and principal methods of dipole moment measurement, as well as an exposition of the criteria employed in selecting the tabulated data.

Key Words: Dielectric constant, electric dipole moments, gas phase, microwave, microwave absorption, molecular beam, permittivity, refractive index, spectroscopy.

1. Introduction

This table of selected values of electric dipole moments for molecules in the gas phase was prepared under a program for the critical evaluation of the data of science and technology sponsored by the National Bureau of Standards through the National Standard Reference Data System. The table revises and brings up to date the data on dipole moments included in the National Bureau of Standards Circular 537, prepared by A. A. Maryott

and F. Buckley in 1953. It gives a recommended value for each compound and an estimate of the accuracy of this value. The most significant experimental values and the methods used to obtain them are tabulated, as well as a complete list of references. Where precise information on two or more vibrational states or isotopic species is available, it has been included in supplemental tables in the appendices.

2. Arrangement and Explanation of Table

2.1. Ordering of Compounds

Compounds are divided into two groups: (a) those containing no carbon atoms (inorganic), arranged with the elemental symbols of the empirical formulas in alphabetical order, and listed alphabetically, and in ascending order of the empirical formula subscripts; (b) compounds containing carbon, ordered as in (a) with the exceptions that carbon is listed first and hydrogen second. Monatomic and homonuclear diatomic molecules, which have no dipole moment in the ground electronic state because of symmetry considerations, are not included.

2.2. Nomenclature

The recommendations of the International Union of Pure and Applied Chemistry Reports on Symbolism and Nomenclature published in *J. Am. Chem. Soc.* **82**, 5517-84 (1960), are followed. The common, or trivial, names are sometimes included in parentheses.

2.3. Units and Corrections

Values of the dipole moment, μ , are expressed in the cgs system of units, since this is the system universally used by workers in the field. The

numerical values are in debye units, D, ($1 \text{ D} = 10^{-18}$ electrostatic units of charge \times centimeters). The conversion factor to the Système International is $1 \text{ D} = 3.33564 \times 10^{-30}$ coulomb-meter. 10^{-30}

Appropriate corrections have been made to values reported in the original literature. In particular, dipole moments which were measured relative to some secondary standard (for example, the OCS molecule) have been corrected in accordance with the best current value for the reference dipole moment (0.7124 D in the case of OCS). Corrections have also been made for changes in the fundamental physical constants. In some cases the primary experimental data have been re-analyzed. Therefore, many of the dipole moments listed in this table differ slightly from the values reported by the original authors.

2.4. Selected Moments

The recommended value of the dipole moment of each compound is listed in the column headed *Selected Moment* and is accompanied by a letter code indicating its estimated accuracy. The selected values are arbitrarily rounded off to 0.01 D except for moments less than 1 D, where an additional significant figure has been given when warranted. The accuracy code and related notation are given in the following table; a discussion of the basis for assigning the reliability is given in section 6.

Code symbol	Estimated accuracy of value
A	$\pm 1\%$ or, for $\mu < 1.0$ D, ± 0.01 D
B	$\pm 2\%$ or, for $\mu < 1.0$ D, ± 0.02 D
C	$\pm 5\%$ or, for $\mu < 1.0$ D, ± 0.05 D
D	$\pm 10\%$ or, for $\mu < 1.0$ D, ± 0.10 D
Q	Questionable value
S	$\mu \equiv 0$ on grounds of molecular symmetry
i	The significance of these values may involve some ambiguity because of the possibility of different conformations or spatial isomers.

The Q code symbol has been used where there is a serious question about the best value to select or where there is insufficient information on which to base a meaningful estimate of accuracy. The symbol is also used when only one component of the dipole moment vector has been measured. All values in this category have been placed in parentheses to emphasize their questionable nature. They may be regarded as giving a rough estimate of the magnitude of the moment but are not of sufficient accuracy for quantitative use. The symbol xQ, without a numerical value being given, indicates that the reported values of the dipole moment are so doubtful that they could be misleading. When the symbol i appears without a numerical value, it indicates the probable presence, in significant amounts, of two or more conformational isomers which may have quite different dipole moments. In such cases the average moment and its temperature dependence are indicated in a footnote.

Further discussion regarding the definition and significance of the dipole moment, the experimental

methods for its determination, and the criteria for evaluation of the data may be found in sections 4, 5, and 6.

2.5. Basic References

The column headed *Basic References* lists the reference number to the Bibliography (sec. 8), the experimental method, and the dipole moment (in that order) of all sources that were taken into consideration in arriving at the selected value and the estimate of its accuracy. The method code is

- MW = microwave spectroscopy
 MB = molecular beam electric resonance
 DT = permittivity (dielectric constant) as a function of temperature
 DR = permittivity and refractive index data
 NR = nonresonant microwave absorption or dispersion
 ↗ = an arrow following the listed value of the moment indicates that the reference contains information about its orientation relative to the molecular framework.

2.6. Other Data

The last column lists additional references not used in obtaining the selected value. These include published reports of a preliminary nature, other articles which contain essentially the same information as in the *Basic References*, or work considered to be of lesser reliability. Reference to supplemental information contained in the appendices is noted by

- Vib—refers to data on dipole moments in excited vibrational states (appendix I)
 Iso—refers to data on dipole moments of different isotopic species (appendix II).

3. Bibliographic Compilation Procedure

A number of literature searches for information on dipole moments have previously been carried out. We have made use of these in collecting the bibliography on which the present table is based. The following compilations were particularly helpful:

Tables of Experimental Dipole Moments by A. L. McClellan (W. H. Freeman and Co., San Francisco, 1963).

Tables of Dielectric Constants and Electric Dipole Moments of Substances in the Gaseous State by A. A. Maryott and F. Buckley (U.S. National Bureau of Standards Circular 537, 1953).

Digest of Literature on Dielectrics, 29 volumes (National Academy of Sciences-National Research Council publication, annual) (order from the Staff Executive, Conference on Electrical Insulation, N.A.S.-N.R.C., 2101 Constitution Ave., NW., Washington, D.C. 20418).

Microwave Spectral Tables NBS Monograph 70 (Diatomic Molecules, Vol. 1) by P. F. Wacker, M. Mizushima, J. D. Peterson, and J. R. Ballard (U.S. Government Printing Office, 1964).

Microwave Gas Spectroscopy Bibliography 1954-1964, by Paolo G. Favero (Laboratorio di Spettroscopia a Radiofrequenza, University of Bologna, Bologna, Italy, 1963, 1966).

Bibliographie mikrowellenspektroskopischer Untersuchungen an Molekülen in den Jahren 1945-1962 by B. Starck (Physikalisches Institut der Universität, Freiburg i. Br., Germany, 1963).

Table of Electric Dipole Moments by L. G. Wesson (The Technology Press, Cambridge, Mass., 1948).

Landolt-Börnstein Tabellen (6 Auflage) (1951) Parts 142061-142063 (H. Stuart).

Microwave Spectroscopy by C. H. Townes and A. L. Schawlow (McGraw-Hill Book Co., Inc., New

York, 1955) Appendix VI (by G. C. Dousmanis).

Molecular Microwave Spectra Tables by P. Kisliuk and C. H. Townes (U.S. National Bureau of Standards Circular 518, 1952).

Table of Electric Dipole Moments by S. Crompton, Master's Thesis, Duke Univ. (Durham, N.C., 1948).

Several of the above compilations were based on comprehensive searches of *Chemical Abstracts* and similar sources. As a result of this overlap, we may have a high degree of confidence that very few references have been overlooked. This conclusion was supported by a check of the 1952 and 1953 *Chemical Abstracts* in which no new references were uncovered. A certain number of incorrect or irrelevant references were discovered in previous compilations. These have been corrected or eliminated in the present bibliography.

The bibliography has been limited, as far as possible, to the regular published literature. References to theses, reports, abstracts of meetings, and private communication are included in only a few

cases where they cover important data which are not otherwise available. Certain preliminary notes on results which were later published in more detail have also been excluded.

An effort has been made to provide complete coverage of the literature through the end of 1965. Some references to papers appearing in 1966 are also included, but the coverage for this year is not complete.

The bibliography (sec. 8) is ordered primarily by year of publication, secondarily by the first-named author's last name, and finally by the next-named authors. The references are numbered serially, the most recent references having the highest numbers. Since some additions and deletions in the bibliography were made prior to publication of the tables, there are several reference numbers which are unused, and several 1966 references are not ordered according to the above scheme. The journal names have been abbreviated according to the 1961 listing in *Chemical Abstracts*.

4. Definition of Dipole Moment

We have attempted in this tabulation to select the best value of the dipole moment of each compound on which measurements have been made. Some discussion is therefore in order concerning the extent to which the electric dipole moment can be considered a well-defined molecular property. The permanent dipole moment of an isolated molecule is normally defined as

$$\boldsymbol{\mu} = \left\langle \sum_i e_i \mathbf{r}_i \right\rangle, \quad (1)$$

where the summation extends over all charges e_i (nuclei and electrons) in the molecule. The position vectors \mathbf{r}_i may be referred to any origin as long as the molecule has no net charge. Since the expectation value in eq (1) implies a particular stationary state, an important question arises concerning the dependence of $\boldsymbol{\mu}$ on rotational, vibrational, and electronic state. At present there is no evidence of significant variation of dipole moment with rotational state. The variation with vibrational state would be expected to be larger, and, indeed, changes of 1 to 2 percent per quantum of vibrational excitation have been observed (see appendix I). The dependence on electronic state is much more critical; changes of 30 percent or more have been reported (see CH_2O). Another source of variation lies in isotope effects. Replacement of hydrogen by deuterium has been found to change dipole moments by several percent in some cases. However, for atoms other than hydrogen, the effect is very much smaller (see appendix II).

In view of these considerations we have chosen to define the dipole moment of a compound as the

moment of a molecule of the dominant isotopic species of that compound in its ground electronic and vibrational state. The selected values in the present table are, in principle, based on this definition. This allows the dipole moment of a compound to be uniquely specified, at least to the extent that the influence of molecular rotation can be ignored. Dipole moments determined by spectroscopic methods (see sec. 5) always refer to a particular vibrational and electronic state and to a single isotopic species; the present definition is therefore the most convenient one to use when dealing with spectroscopic results. However, moments determined from measurements of bulk dielectric properties represent an average over the equilibrium population of vibrational (and, in principle, electronic) states and over the natural abundance of the various isotopic species. While this introduces a certain ambiguity in the comparison of moments determined by the two methods, an examination of the best available data indicates that the distinction is of little practical importance except in special cases. That is, the average moment determined from bulk dielectric properties at ordinary temperatures is unlikely to differ by more than 1 percent from the moment of the dominant isotopic species in its ground state.

Certain difficulties do arise in comparing spectroscopic and dielectric results on molecules which can rapidly interconvert between spatially distinct forms. For example, two conformational isomers of a compound may have quite different dipole moments. Spectroscopic measurements permit the moments of the individual isomers to be determined, while dielectric measurements yield an average moment appropriate to a particular tem-

perature. Where spectroscopic results were available, we have treated such conformational isomers as separate compounds and listed the individual dipole moments in the table. However, where there were only dielectric measurements, an average moment has been listed with a notation

that conformational isomers are probably present; information on temperature dependence of the average moment is given in footnotes. The problem of dealing with conformational isomerism is discussed in more detail in sections 5 and 6.

5. Principal Methods of Dipole Moment Measurement

5.1. Microwave Spectroscopy (MW)

When a polar molecule is placed in an external electric field of magnitude E , the rotational energy levels of the molecule are split through the Stark effect. If the total angular momentum of the molecule in the absence of the field is described by the quantum number J , application of the field results in $2J+1$ states which are designated by a quantum number $M=J, J-1, \dots, -J$. In the most common case, where the Stark splitting can be adequately described by second-order perturbation theory, the correction ΔW to the rotational energy has the form

$$\Delta W = (A + BM^2)E^2. \quad (2)$$

Thus each rotational level splits into $J+1$ distinct sublevels, and the magnitude of this splitting is quadratic in the applied field. For easily obtainable laboratory fields the splitting is large enough to be resolved in pure rotational transitions observed in the microwave region of the spectrum. Measurement of the splitting of a spectral line as a function of the applied field allows an accurate determination of the coefficients A and B in eq (2).

The A and B coefficients depend upon the dipole matrix elements connecting the level in question with all other rotational levels and upon the corresponding energy separations. If the dipole moment μ is resolved into components μ_g along suitable molecule-fixed axes (usually the principal inertial axes a, b, c), each dipole matrix element may be written as the product of μ_g times a matrix element of a direction cosine between the molecule-fixed and external axis systems. A complete analysis of the microwave spectrum provides enough information to calculate the direction cosine matrix elements by well-known methods; likewise, the energy-level separations can be accurately calculated. It is therefore possible to extract the dipole components μ_g from the experimentally determined A and B coefficients.

A special case arises when degeneracies exist among the rotational levels. If the degenerate levels are connected by a dipole matrix element, a first-order Stark effect occurs which is of the form

$$\Delta W = \pm CME. \quad (3)$$

The coefficient C is proportional to μ_g and can be readily calculated. Degeneracies which lead to

first-order Stark effects occur systematically in symmetric-top molecules, and they are frequently present in asymmetric rotors as well. When there is a near, but not exact, degeneracy, the Stark effect may be neither linear nor quadratic but can have a more complicated form.

The first and second-order Stark perturbation terms are almost always sufficient to permit a measurement of the dipole moment with an uncertainty of 1 percent or less. However, for more accurate work, and in a few special cases, higher order terms must be considered. The next important terms are the fourth-order contribution from the permanent dipole moment and the second-order contribution from the induced moment. These may be of comparable magnitude. In calculating direction cosine matrix elements and energy separations it is sometimes necessary to take centrifugal distortion into account.

The microwave method of measuring dipole moments offers many advantages. Determination of the moment with an uncertainty of 1 percent (which requires that the Stark splittings be measured to within only 2 percent if the Stark effect is second-order) can generally be done without particular difficulty. The same percentage accuracy is possible with small moments, even those less than 0.1 D. The purity of the sample is not important. The measurement is made on a specific vibrational state and isotopic species, so that variation of the moment with these factors can be studied. Where two or more rotational isomers are present in significant concentrations, their moments may be individually measured. Finally, since the separate components of the dipole moment vector are determined, information is available on the orientation of the moment relative to the molecular framework.

In spite of these advantages, a fair number of dipole moments measured by the microwave method are not accurate to within 1 percent, and the uncertainty is quite large in some reported values. There are several reasons for this. Many spectra are complicated by nuclear quadrupole hyperfine structure, which introduces another perturbation which may be comparable in magnitude to the Stark effect. If the Stark shifts can be made much larger or much smaller than the hyperfine structure, the analysis is fairly straightforward, and the accuracy of measurement should be as high as when hyperfine structure is absent. In the intermediate case, however, the analysis of the data is more compli-

cated, and misleading results can be obtained unless the calculations are done very accurately. In some of the earlier microwave measurements this problem does not appear to have been sufficiently appreciated, and the resulting dipole moments are correspondingly less reliable.

Another difficulty sometimes arises when the Stark effects of all accessible transitions are sensitive to one dipole component but quite insensitive to the others. Thus only one component can be determined with high accuracy, and the total moment is subject to a sizable uncertainty. A high density of lines in the spectrum also presents problems, since it is sometimes difficult to avoid the overlapping of Stark components from different lines.

The accuracy of a dipole moment determined from the Stark effect is dependent, of course, on the measurement of the electric field strength. While there is no problem in measuring the applied voltage accurately, the effective spacing between electrodes is not so easily determined. This problem has been discussed in several places (222, 360, 712). It has become common practice to calibrate the effective electrode spacing by measuring the Stark effect of the OCS molecule, whose dipole moment is accurately known. Most of the dipole moments determined by the microwave method have, in fact, been measured relative to OCS. In view of this practice, it seems highly desirable to use OCS as the primary standard for field-strength calibration whenever possible, in order that all reported moments be on a common basis.

The most accurate determination of the OCS dipole moment is that of Marshall and Weber, who obtained 0.7124 D. Independent measurements in other laboratories indicate that the uncertainty of this value is no greater than 0.1 percent. Other convenient molecules for use as secondary standards are CH₃CN (3.918 D), CH₃F (1.847 D), and CHF₃ (1.646 D). These values should be accurate to within at least 0.5 percent. Full references to these compounds may be found in the main table.

5.2. Molecular Beam Electric Resonance (MB)

This method is very similar in principle to that discussed under microwave spectroscopy, since it makes use of the Stark effect of rotational transitions. However, the measurement is carried out on a molecular beam, where the spectral line widths are much smaller, and the accuracy with which the Stark splittings can be measured is greatly improved. Furthermore, the apparatus can be designed so that the electric field is more uniform and its absolute value more accurately measureable than is possible in the normal micro-

wave absorption cell. The transitions which are studied can lie anywhere in the radiofrequency or microwave regions. It is thus possible to measure the Stark splittings within a single rotational level as well as the Stark effect of rotational transitions. The accuracy is usually greater for the former measurement; however, in order to extract the dipole moment from the Stark splittings it is necessary to know accurately the spacing between rotational levels. This may be determined by measurement of rotational transitions, either by beam techniques or by conventional microwave spectroscopy. Some very accurate dipole moments have been derived from a combination of molecular beam measurements in the radiofrequency region and conventional microwave measurements of rotational transitions.

The molecular beam technique offers the highest inherent accuracy of any known method of dipole moment determination. Uncertainties approaching 0.02 percent have been claimed by some investigators, and the precision is an order of magnitude higher than this. It is thus possible to detect very small changes of dipole moment with vibrational state and isotopic species.

The chief limitation of the molecular beam technique is the very restricted class of molecules to which it can be applied. Practically all measurements reported so far have been on diatomic molecules, except for a very few triatomics. This limitation results from the fact that the population is distributed over a large number of states in more complicated molecules, with a resulting loss of sensitivity.

A few early measurements of dipole moments were based on the deflection of molecular beams by static electric fields (017, 018, 086, 107, 114, and other references). This is a much cruder technique than the electric resonance method discussed above, since the measurements were of limited accuracy and there was little control of the constitution of the beam. Determinations of this type have been given no weight in the present tabulation, but the references are included in the *Other Data* column.

5.3. Dielectric (DT, DR, NR)

Prior to the development of microwave and molecular beam techniques in the late 1940's, the more reliable determinations of dipole moments were all based upon application of the Debye equation to measurements of the low frequency, or "static" permittivity (dielectric constant). The molar polarization, P , is defined by

$$P = \frac{\epsilon - 1}{\epsilon + 2} V = \frac{4\pi N\alpha}{3} + \frac{4\pi N\mu^2}{9kT} = A + \frac{B}{T} \quad (4)$$

where

ϵ = permittivity (dielectric constant)
 V = molar volume
 α = molecular polarizability (electronic plus vibrational)
 N = Avogadro's number
 k = Boltzmann's constant
 T = temperature, absolute ($^{\circ}\text{K}$).

Equation (4) has been used in two ways, one direct and the other indirect, to derive values for the dipole moment. Recently a third procedure, based on measurements of the complex permittivity (dispersion or absorption) at the lower microwave frequencies, has been used to a limited extent. The latter method is limited primarily to symmetric top molecules (symmetry C_{nv} with $n \geq 3$).

5.4. Temperature-Variation Procedure (DT)

In this method P is measured as a function of $1/T$ and the dipole moment obtained from the slope B and the relation

$$\mu = 0.01281 (B)^{1/2},$$

if B is given in $\text{cm}^3 \text{mol}^{-1} \text{ } ^{\circ}\text{K}$. This is the direct and preferred procedure, but it requires precise data over an extended temperature range. In addition the mean squared moment, averaged over the thermal distribution of vibrational and rotational states must be essentially independent of temperature. Under favorable conditions, values accurate to within 1 percent are obtained.

5.5. Indirect (Optical) Procedure (DR)

In some instances available data are either limited to one temperature or are of limited precision and scope and do not permit a reliable determination of B . The substance may, for example, have a low volatility and restricted range of thermal stability. In other cases there may be an equilibrium between different conformational isomers with different dipole moments which is temperature dependent. An effective dipole moment is then computed for any given temperature by

$$\mu = 0.01281 [(P-A)T]^{1/2} \quad (5)$$

with an assumed value for A . Since direct knowledge of the vibrational contribution to the polarization is generally lacking, various arbitrary or empirical assumptions have been made. Sometimes the vibrational polarization is taken as a fixed percentage of the electronic contribution (e.g., 5, 10, or 15 percent). Theoretically, however, the vibrational and electronic polarizations are unrelated.

The most common convention has been to ignore the vibrational contribution to the polarizability and to replace A by the molar refraction, R_D , for the sodium line. If R_D is not known directly, it can usually be estimated with sufficient reliability (especially for organic compounds) by summing tabulated atomic or bond refractions. Then

$$\mu \leq 0.01281 [(P-R_D)T]^{1/2}, \quad (6)$$

since this convention tends to set an upper limit to the value for the dipole moment consistent with the experimental data. Equation (6) is used in the present tabulation unless otherwise noted. In structurally simple molecules with relatively large dipole moments, the uncertainty in the use of Equation (6) may be less than 2 percent.

5.6. Nonresonant Microwave Absorption or Dispersion (NR)

This method is applicable in special cases where there are nonvanishing dipole matrix elements connecting degenerate or nearly degenerate rotational states, in particular symmetric-top molecules. The resulting absorption and dispersion are characterized by a relaxation, or Debye-type, spectrum. By suitable choice of frequencies and pressures, this spectrum can be observed without significant interference from the ordinary rotational spectrum. Details of the method applied to absorption are contained in references [337] and [343] of the Bibliography and in reference [416] for the case of dispersion. In essence, the method enables one to obtain a fractional part of the total dipolar polarization in eq (4), namely fB/T , the fraction f being readily computed provided the moments of inertia are known. The method is particularly useful for substances with very small values of the dipole moment. Values as low as 0.1 D may be determined with an uncertainty of the order of 2 percent, and values much smaller than this may be determined with somewhat poorer accuracy.

5.7. Comments on Dielectric Methods

Compared to the spectroscopic techniques, the dielectric methods have certain limitations and disadvantages. Since they involve bulk property measurements, substances of high purity and chemical stability are required and the experimental variables, density and temperature, must be accurately known. In addition the derived moments represent averages over the various molecular states of the system and, as noted previously, cannot be as precisely defined as the spectroscopic values. For relatively simple rigid molecules this ambiguity is probably trivial for most purposes. This is borne out by intercomparison of results in

the more favorable cases where the value of the dipole moment is greater than one debye. In such cases agreement between the spectroscopic and dielectric (DT) methods is usually of the order of 1-2 percent, the differences being comparable with the overall experimental uncertainties.

Dielectric methods, on the other hand, have frequently been applied to molecules of greater molecular complexity than those ordinarily studied by spectroscopic methods. In many instances such molecules can exist, at least in principle, in two or more spatial conformations with different dipole moments. The analysis and interpretation in such cases may be somewhat arbitrary, depending on intuitive judgment or additional independent information. We may define two rather limiting situations.

(I) The molar polarization varies with temperature but definitely not in the manner shown explicitly by eq (4), so that $\langle \mu^2 \rangle$ is a function of temperature. Simple examples are the 1,2-disubstituted ethanes (XCH_2CH_2X') which exist in equilibrium mixtures of "trans" (nonpolar if $X = X'$) and dipolar "gauche" isomers.

(II) The polarization varies inversely with T and gives a reasonable value for the intercept A so that there appears to be no significant variation of $\langle \mu^2 \rangle$ with T . Alternative interpretations of case II are: (a) only one conformation exists to a significant extent over the temperature range of observation, (b) the different conformations have essentially the same dipole moment, (c) differences in energies of the various conformations are small and the equilibrium distribution insensitive to temperature.

6. Criteria for Evaluation

The evaluation of the data on dipole moments was carried out in two stages. It was first necessary to assess the accuracy of results obtained by each experimental technique and to rationalize discrepancies in duplicate measurements by the same method. This was done for each compound by an evaluator who was familiar with the particular technique. Secondly, in cases where results had been reported by more than one technique, a decision had to be made on the final selected value and its accuracy. The factors which were taken into account in the evaluation process are discussed below.

6.1. Microwave Measurements

When the original investigator has given an uncertainty with his dipole moment value (and this is not always the case), this fact has been taken into consideration. However, the primary data have also been examined whenever they were published in order to obtain some independent feeling for the overall accuracy of the measurement. The following factors were taken into account:

1. Number of Stark components whose shifts were measured.
2. Number of data points for each component.
3. Scatter of these data points.
4. Range of frequency shifts.
5. Internal consistency among the different components (when the number of components measured was greater than the minimum required for the dipole moment determination).
6. Approximations used in the Stark effect calculation.
7. Complicating effects such as hyperfine structure and internal rotation (and the degree to which these effects were considered in the calculations).

8. Method of calibration of field strength.

Consideration of the above factors gave some feeling, at least in a subjective way, of the confidence which could be placed in the reported dipole moment. In addition, the general pattern of results from a given laboratory during a given period was studied. When comparisons could be made on molecules which were subsequently remeasured with greater accuracy, it sometimes became obvious that the original error estimates were too low. These observations were taken into account in the assignment of reliability to results obtained in that laboratory.

Unfortunately, many papers do not give enough details for a meaningful evaluation to be made. This is particularly true in abstracts and short notes published during the 1945-50 period. In such cases the evaluators have been conservative in estimating the reliability.

6.2. Molecular Beam Measurements

The uncertainty in most dipole moments measured by molecular beam techniques is appreciably less than 1 percent (see sec. 5). These values have been placed in category A, and no further evaluation has been made. In one or two cases where discrepancies of more than 1 percent occur between duplicate measurements, the more recent results have been accepted.

6.3. Dielectric Methods

Only a few values of dipole moments have been reported from the study of nonresonant spectra (NR). These have usually been obtained from measurements of the imaginary part of the complex permittivity (loss index, ϵ'') but occasionally from

the dispersion of the real part, ϵ' . Precise resonant cavity techniques, which should be relatively free of systematic errors, have been used. The method has been applied primarily to substances having dipole moments substantially less than 1 D. The accuracy of these values are generally regarded as in the A or B categories.

In the case of low frequency measurements of permittivity, the original data have been reexamined to determine, in the opinion of the evaluator, the best procedure for analysis (DT or DR). Preference has been given to the temperature-variation procedure (DT), where warranted by the precision and scope of the data, where there appeared to be no thermal decomposition, and where there was no evidence that the effective dipole moment varied with temperature. In these cases values of A and B (eq (4)) were obtained by the method of least squares, if this was not done in the original reports.

Values analyzed by the indirect procedure (DR) were recomputed, where necessary, to conform to the present convention (i.e., $A=R_D$). Values averaged over the temperature range are listed. If there appears to be a significant variation of dipole moment with temperature, no value is listed in the main table. The effective values obtained at the extreme ends of the temperature range are then given in footnotes.

The above procedures were used in the previous tabulation, NBS Circular 537, and most of the values included in the Basic References during the period prior to 1953 are identical with these. In some instances, however, a reconsideration of the data has led to a change in the method of analysis. It should be emphasized that the dipole moment attributed to a given reference is not necessarily the same as the value originally reported, either because of a difference in our treatment of the data or because of the small corrections to the moments resulting from changes in the values of the physical constants.

In estimating accuracy consideration is given to various factors such as

1. Chemical purity.
2. Scope and precision of data (statistical precision index in least squares for DT method).
3. Likely uncertainty in use of DR method due to neglect of vibrational polarization (depending on molecular type and magnitude of the moment).
4. Overall consistency and agreement of work in given laboratory with reliable, independently established data.

6.4. Choice of Selected Moments

In many cases where results on the same compound had been obtained by more than one method

there was a fairly obvious choice of the most accurate value. For example, with moments less than about 0.5 D microwave (MW) values are known to be significantly more accurate than DR or DT values. In other cases the microwave determination was complicated by hyperfine structure or other factors, and the dielectric values were clearly more reliable. In such situations the selection of the best value was fairly straightforward. In other cases different values of comparable reliability were in agreement within their estimated uncertainties. Here an average value was adopted, weighted in favor of the method which seemed more accurate. Finally, there were a few compounds for which unresolved discrepancies existed between the moments obtained by two techniques. In such cases an average was taken, and an uncertainty which was large enough to include both values was assigned.

We feel that this procedure leads to the most meaningful set of selected values which can be obtained from a collection of data from such diverse sources. However, it is obvious that no well-defined statistical estimator can be assigned to specify the uncertainty of the final selected value. We have therefore used an accuracy code A, B, C, D to indicate the limits within which, in our best judgment, the selected value can be trusted. The code is explained in section 2. If a value is placed in category A, for example, it can be concluded with high confidence that the true dipole moment does not differ by more than 1 percent from the value given (or by more than 0.01 D, in case of moments less than 1 D).¹ While this procedure involves many subjective factors and rests heavily on the judgment of the evaluators, it is felt to be the most useful way of presenting the results.

Where the selected value is based solely on dielectric methods, and the presence in significant amounts of two or more conformational isomers is possible, the value is followed by the symbol *i*. Such values are conditional in two respects: (a) if only one conformation is present in significant amounts, independent data may be needed to specify the particular conformation; and (b) the dipole moment may be more uncertain than suggested by the reliability code because of a small, but not obvious, variation of $\langle \mu^2 \rangle$ with T . Therefore, the interpretation of these dipole moments as specific molecular properties should be made with caution.

¹ It should be pointed out that the uncertainty in some of the A values is appreciably less than 1 percent.

7. Table of selected dipole moments

7.1. Selected moments (compounds not containing carbon)

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
AgCl	Silver chloride.....	5.73 C	580 MW 5.73	
AlCl	Aluminum chloride.....	x Q	564 MW 1 to 2	
AlF	Aluminum fluoride.....	1.53 D	564 MW 1.53	512
AsCl ₃	Arsenic trichloride.....	1.59 C	117 DT 1.59	
AsF ₃	Arsenic trifluoride.....	2.59 B	485 MW 2.61 446 DT 2.57	219,
AsH ₃	Arsine.....	0.20 C	239 MW 0.22 ^a 016 DT 0.16	
As ₂ O ₃	Diarsenic trioxide.....	x Q	028
BCl ₃	Boron trichloride.....	0 S	298 DT 0	117
BF ₃	Boron trifluoride.....	0 S	115 DT 0 123 DT 0	
B ₂ H ₆	Diborane.....	0 S	102 DT 0	
B ₃ H ₆ N ₃	Triborotriazine (Borazine).....	0 S	102 DT 0.7 ^b	
B ₅ H ₉	Pentaborane.....	2.13 B	294 MW 2.13	259
BaO	Barium oxide.....	7.95 A	526 MB 7.954	500, Vib
BrCl	Bromine chloride.....	(0.6) Q	224 MW 0.57	
BrF	Bromine fluoride.....	(1.3) Q	223 MW 1.29	
BrF ₃	Bromine trifluoride.....	(1.1) Q	358 MW 1.0 326 DR 1.19	
BrF ₅	Bromine pentafluoride.....	1.51 D	339 DT 1.51	
BrH	Hydrogen bromide.....	0.82 B	007 DT 0.80 392 MW 0.83 ^c	
BrH ₃ Si	Bromosilane.....	1.33 B	265 MW 1.33	217
BrK	Potassium bromide.....	10.41 B	274 MB 10.41	114, 107, Vib
BrLi	Lithium bromide.....	7.27 A	535 MB 7.2680 ^d	293, Vib, Iso
BrNO	Nitrosyl bromide.....	(1.8) Q	579 MW 1.80 ^e	396
BrRb	Rubidium bromide.....	x Q	017
Br ₂ Hg	Mercury dibromide.....	0 S	095 DT 0	
Br ₄ Sn	Tin tetrabromide.....	0 S	131 DT 0	
ClCs	Cesium chloride.....	10.42 A	341 MB 10.42	284, 241, 017, Vib
ClF	Chlorine fluoride.....	0.88 C	190 MW 0.881	

^a For ¹H₂ ²H⁷⁵As.

^b The finite reported value is probably due to thermal instability.

^c For ²H⁷⁹Br.

^d For ⁷⁹Br⁶Li.

^e Component along *a* axis.

7.1. Selected moments (compounds not containing carbon)–Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
ClFO ₃	Perchloryl fluoride.....	0.023 A	361 NR 0.023 595 MW ^a 0.025	335, 565
ClF ₃	Chlorine trifluoride.....	0.6 D	326 DT 0.65 336 DT 0.56	264
ClGeH ₃	Chlorogermane.....	2.13 A	265 MW 2.13 ^b 150 DR 2.03	188
ClH	Hydrogen chloride.....	1.08 B	128 DT 1.08 050 DT 1.08 007 DT 1.05 344 DT 1.10 392 MW 1.12	067, 015, 005, 006
ClH ₃ Si	Chlorosilane.....	1.31 A	265 MW 1.310 129 DT 1.29	189, 188, 215
ClI	Iodine chloride.....	(0.6) Q	181 MW ^a 0.65 073 DT 0.54	
ClK	Potassium chloride.....	10.27 A	282 MB 10.48 306 MW 10.1 591 MB 10.2688	086, 114, 107, Vib
ClLi	Lithium chloride.....	7.13 A	537 MB 7.1195 ^c 591 MB 7.1289 ^c	Vib, Iso
ClNa	Sodium chloride.....	9.00 A	306 MW 8.5 473aMB 9.002	Vib
ClNO	Nitrosyl chloride.....	(1.9) Q	391 MW 1.86 ^d	244
ClNO ₂	Nitryl chloride.....	0.53 A	579 MW 0.53 393 MW 0.53	386
ClTl	Thallium chloride.....	4.44 B	254 MB 4.444 379 MW 5.1	
Cl ₂ F ₃ P	Dichlorotrifluorophosphorus.....	0.68 C	561 DT 0.68	
Cl ₂ H ₂ Si	Dichlorosilane.....	1.17 B	129 DT 1.17	
Cl ₂ Hg	Mercury dichloride.....	0 S	095 DT 0	

^a Calculated from microwave intensities.

^b For ³⁷Cl⁷⁴Ge¹H₃.

^c For ³⁵Cl⁶Li.

^d Component along *a* axis.

7.1. Selected moments (compounds not containing carbon)—Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
Cl ₂ OS	Thionyl chloride.....	1.45 B	143 DT 1.45	
Cl ₂ O ₂ S	Sulfuryl chloride.....	1.81 B	143 DT 1.81	
Cl ₃ F ₂ P	Trichlorodifluorophosphorus.....	0 S	561 DT 0	
Cl ₃ HSi	Trichlorosilane.....	0.86 B	129 DT 0.86	
Cl ₃ P	Phosphorus trichloride.....	0.78 C	072 DT 0.78	
Cl ₄ FP	Tetrachlorofluorophosphorus.....	0.21 B	567 NR 0.21	
Cl ₄ Ge	Germanium tetrachloride.....	0 S	131 DT 0	
Cl ₄ Si	Silicon tetrachloride.....	0 S	298 DT 0	
Cl ₄ Sn	Tin tetrachloride.....	0 S	131 DT 0	
Cl ₄ Ti	Titanium tetrachloride.....	0 S	131 DT 0	
CsF	Cesium fluoride.....	7.88 A	341 MB 7.875	293, 203, 167, 169, 192, Vib
CsI	Cesium iodide.....	x Q	114, 107
FH	Hydrogen fluoride.....	1.82 A	525 MB 1.8195 163 DT 1.91 176 DT 1.91 532 MB 1.83	465, 462
FH ₃ Si	Fluorosilane.....	1.27 B	218 MW 1.268	
FH ₅ Si ₂	Fluorodisilane.....	1.26 A	578 MW 1.26 ↗	
FK	Potassium fluoride.....	8.60 A	421 MB 8.60	210
FLi	Lithium fluoride.....	6.33 A	527 MB 6.328 ^a 591 MB 6.325	309, Vib, Iso, 268
FMnO ₃	Permanganyl fluoride.....	(1.5) Q	296 MW 1.5 ^b	
FNO	Nitrosyl fluoride.....	1.81 B	242 MW 1.81 ↗	
FNO ₂	Nitryl fluoride.....	(0.47) Q	267 MW 0.47	
FNa	Sodium fluoride.....	8.16 A	536 MB 8.1558 528 MB 8.19	501, Vib
FO ₃ Re	Perrhenyl fluoride.....	0.85 D	406 MW 0.85 ^b	385
FRb	Rubidium fluoride.....	8.55 A	382 MB 8.80 591 MB 8.5465	Vib
FTl	Thallium fluoride.....	4.23 A	397 MB 4.2282 379 MW 3.99	374, 380, Vib, Iso
F ₂ HN	Difluoramine.....	1.92 A	513 MW 1.921 ↗	
F ₂ H ₂ Si	Difluorosilane.....	1.55 A	353 MW 1.55	
F ₂ N ₂	<i>cis</i> -Difluorodiazine.....	0.16 A	510 MW 0.16	
F ₃ O	Oxygen difluoride.....	0.297 A	460 MW 0.297 419 DR 0.4	417

^aFor ¹⁹F⁶Li.

^bIn excited vibrational state $v_3=1$.

7.1. Selected moments (compounds not containing carbon) – Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
F ₂ OS	Thionyl fluoride.....	1.63 A	290 MW 1.627 ↗	256
F ₂ O ₂	Dioxygen difluoride.....	1.44 C	478 MW 1.44	
F ₂ O ₂ S	Sulfuryl fluoride.....	1.12 B	355 MW 1.116	
F ₂ S ₂	Sulfur monofluoride (S=SF ₂ isomer).....	1.03 C	536aMW 1.03 ↗	
F ₂ S ₂	Sulfur monofluoride (FSSF isomer).....	1.45 B	536aMW 1.45	
F ₂ Si	Silicon difluoride.....	1.23 B	571 MW 1.23	
F ₃ HSi	Trifluorosilane.....	1.27 B	275 MW 1.27	
F ₃ N	Nitrogen trifluoride.....	0.235 A	297 MW 0.236 275 MW 0.235 ^a 115 DT 0.25 102 DT 0.22	
F ₃ NS	Nitridotrifluorosulfur.....	1.91 B	481 MW 1.91	
F ₃ OP	Phosphoryl fluoride.....	1.76 B	275 MW 1.78 258 MW 1.70 216 MW 1.735	
F ₃ P	Phosphorus trifluoride.....	1.03 A	275 MW 1.03 219 MW 1.030	
F ₃ PS	Thiophosphoryl fluoride.....	0.64 B	258 MW 0.636	
F ₄ N ₂	Tetrafluorohydrazine, <i>gauche</i> conformation.....	0.26 B	405 MW 0.26	
F ₄ S	Sulfur tetrafluoride.....	0.632 A	498 MW 0.632 419 DR 1.0	
F ₄ Si	Silicon tetrafluoride.....	0 S	094 DT 0	
F ₅ P	Phosphorus pentafluoride.....	0 S	123 DT 0	
F ₅ I	Iodine pentafluoride.....	2.18 C	326 DR 2.18	149, 133
F ₆ S	Sulfur hexafluoride.....	0 S	546 DT 0 446 DT 0 094 DT 0	
F ₆ Se	Selenium hexafluoride.....	0 S	
F ₆ Te	Tellurium hexafluoride.....	0 S	149
F ₆ U	Uranium hexafluoride.....	0 S	336 DT 0 243 DT 0 171 DT 0	
F ₁₀ S ₂	Disulfur decafluoride.....	x Q	235
HI	Hydrogen iodide.....	0.44 B	392 MW 0.443 ^b 007 DT 0.42	375, 487a

^a For ¹⁹F₃¹⁵N.

^b For ²H¹²⁷I.

7.1. Selected moments (compounds not containing carbon)–Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
HLi	Lithium hydride.....	5.88 A	442 MB 5.882	462, Vib, Iso
HN	Imidyl radical.....		561b (a)	
HNO ₃	Nitric acid.....	2.17 A	556 MW 2.17 ↗ 435 MW 2.17 ↗	
HN ₃	Hydrogen azide (hydrazoic acid).....	(0.8) Q	205 MW 0.847 ^b	
HO	Hydroxyl radical.....	1.66 A	570 MW 1.660 455 MW 1.65 506 MW 1.60	322, 568a
H ₂ N ₂ O ₂	Nitroamine (nitramide).....	(3.6) Q	522 MW 3.57 ^b	
H ₂ O	Water.....	1.85 A	062 DT 1.85 097 DT 1.84 106 DT 1.84 157 DT 1.85 253 DT 1.85 594 MW 1.85	001, 023, 033a, 044, 091, 092, 173, 174, 178, 179, 197, 209, 252, 539
H ₂ O ₂	Hydrogen peroxide.....	2.2 D	323 MW 2.26	301
H ₂ S	Hydrogen sulfide.....	0.97 A	561aMW 0.974 344 DT 0.98 027 DT 0.92 250 DT 0.89	234, 015
H ₂ Se	Hydrogen selenide.....	x Q	331 MW 0.24 368 MW 0.62	369, 390, 414
H ₃ N	Ammonia.....	1.47 A	230 MW 1.468 013 DT 1.47 096 DT 1.47 170 DT 1.46 182 DT 1.44 342 DT 1.44	168, 161, 561, 001, 016, 040, 078, 493, 047 055
H ₃ P	Phosphine.....	0.58 A	285 MW 0.575 ^c 375 MW 0.576 239 MW 0.55 016 DT 0.55	
H ₃ Sb	Stibine.....	0.12 C	239 MW 0.116 ^d	

^a The following values have been obtained for excited electronic states by observing the Stark effect of the electronic emission spectrum: $\mu(A^3\Pi) = 1.31$, $\mu(c^1\Pi) = 1.70$, $\mu(a^1\Delta) = 1.49$ D.

^b Component along *a* axis.

^c Average for ²H²H₂P and ¹H₂²HP.

^d For ¹H₂²H¹²¹Sb.

7.1. Selected moments (compounds not containing carbon)—Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
H ₄ N ₂	Hydrazine.....	1.75 C	479 MW 1.75	
H ₄ Si	Silane.....	0 S	094 DT 0	
H ₆ OSi ₂	Disilyl ether (disiloxane).....	0.24 B	548 DT 0.24	
H ₆ Si ₂	Disilane.....	0 S	094 DT 0	
H ₉ NSi ₃	Trisilylamine.....	≤ 0.1 D	524 DT ≈ 0	
HgI ₂	Mercury diiodide.....	0 S	095 DT 0	
IK	Potassium iodide.....	x Q	114, 107, 086, 017
ILi	Lithium iodide.....	7.43 A	552 MB 7.4285 ^a	293, Vib
INa	Sodium iodide.....	x Q	086, 017
ITl	Thallium iodide.....	x Q	017
I ₄ Sn	Tin tetraiodide.....	0 S	131
NO	Nitrogen monoxide (nitric oxide).....	0.153 A	376 MW 0.158 407 NR 0.148 094 DT 0.16	075
NO ₂	Nitrogen dioxide.....	0.316 A	508 MW 0.316 533 MW 0.294 ^b 139 DT 0.29 081 DT 0.39	116
N ₂ O	Dinitrogen oxide (nitrous oxide).....	0.167 A	219 MW 0.167 187 MW 0.16 094 DT 0.17 083 DT 0.14	202, 045, 031, 015
OS	Sulfur monoxide.....	1.55 A	543 MW 1.55	
OS ₂	Disulfur monoxide.....	1.47 B	408 MW 1.47 [↗]	
OSr	Strontium oxide.....	8.90 A	562 MB 8.900	Vib
O ₂ S	Sulfur dioxide.....	1.63 A	231 MW 1.60 487bMW 1.615 126 DT 1.59 213 DT 1.63 344 DT 1.63 013 DT 1.63	566, 015, 010, 001, 003, 240, Vib
O ₃	Ozone.....	0.53 B	286 MW 0.53 209 DT 0.52	279, 260, 236, 330
O ₃ S	Sulfur trioxide.....	0 S	126 DT 0	
O ₄ Os	Osmium tetroxide.....	0 S	149 DT 0	

^a For ¹²⁷I⁶Li.

^b For ¹⁵N¹⁶O₂.

7.2. Selected dipole moments (compounds containing carbon)

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
CBrF ₃	Bromotrifluoromethane.....	0.65 C	314 DT 0.65	
CBr ₂ F ₂	Dibromodifluoromethane.....	0.66 C	314 DT 0.66	133
CClF ₃	Chlorotrifluoromethane.....	0.50 A	434 NR 0.496 451 MW 0.50 343 NR 0.50 314 DT 0.46	475, 450, 209, 133
CClN	Cyanogen chloride.....	2.82 B	219 MW 2.82 ^a	180
CCl ₂ F ₂	Dichlorodifluoromethane.....	0.51 C	076 DT 0.51	209, 133
CCl ₂ O	Carbonyl chloride (phosgene).....	1.17 A	477 MW 1.17 472 DT 1.18 088 DT 1.19	
CCl ₂ S	Thiocarbonyl chloride.....	0.29 C	143 DT 0.29	
CCl ₃ F	Trichlorofluoromethane.....	0.45 C	076 DT 0.45	133
CCl ₃ NO ₂	Trichloronitromethane.....	1.89 C	088 DR 1.89	
CCl ₄	Carbon tetrachloride.....	0 S	298 DT 0 113 DT 0	112, 012, 115
CFN	Cyanogen fluoride.....	2.17 C	523 MW 2.17	439
CF ₂	Carbon difluoride.....	0.46 B	588 MW 0.46	
CF ₂ O	Carbonyl fluoride.....	0.95 A	483 MW 0.95	
CF ₃ I	Iodotrifluoromethane.....	0.92 C	314 DT 0.92 305 MW 1.0	
CF ₃ NO	Trifluoronitrosomethane.....	(0.3) Q	530 DR 0.31	
CF ₃ NO ₂	Trifluoronitromethane.....	1.44 C	576 MW 1.44	
CF ₄	Carbon tetrafluoride.....	0 S	115 DT 0 102 DT 0 546 DT 0	133
CN ₄ O ₈	Tetranitromethane.....	0 S		131
CO	Carbon monoxide.....	0.112 A	375 MW 0.112 344 DT 0.14 094 DT 0.10 182 DT 0.12 027 DT 0.10	019, 015, 002, 004, 558, ^b 487a
COS	Carbonyl sulfide.....	0.712 A	360 MB 0.7124 525 MW 0.7120 222 MW 0.7085 246 MW 0.712 175 DT 0.72 027 DT 0.67	200, 566, 162, 180
COSe	Carbonyl selenide.....	0.73 B	199 MW 0.73	Vib

^a For ¹²C³⁶Cl¹⁴N.

^b $\mu = 1.38 \pm 0.02$ D. in the excited $\alpha^3\Pi$ electronic state.

7.2. Selected dipole moments (compounds containing carbon)– Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
CO ₂	Carbon dioxide.....	0 S	025 DT 0 050 DT 0 125 DT 0	001, 004, 013, 015, 019, 041, 056, 094, 115
CS	Carbon monosulfide.....	1.98 A	324 MW 1.98	
CSTe	Thiocarbonyl telluride.....	0.17 A	291 MW 0.173 ^a	
CS ₂	Carbon disulfide.....	0 S	298 DT 0	112, 031, 027, 045, 048
CHBrF ₂	Bromodifluoromethane.....	1.50 D	133 DR 1.50	
CHBr ₃	Tribromomethane.....	0.99 B	271 DT 0.99	015
CHClF ₂	Chlorodifluoromethane.....	1.42 B	471 MW 1.43 076 DT 1.41	487, 133, 441
CHCl ₂ F	Dichlorofluoromethane.....	1.29 B	076 DT 1.29	133
CHCl ₃	Trichloromethane (chloroform).....	1.01 B	153 DT 1.01 113 DT 1.02	446, 112, 024, 012
CHFO	Formyl fluoride.....	2.02 A	430 MW 2.02 ✓	420
CHF ₃	Trifluoromethane.....	1.65 A	587 MW 1.646 246 MW 1.646 446 DT 1.65 257 MW 1.65 314 DT 1.62 102 DT 1.60	Iso, 191
CHN	Hydrogen cyanide.....	2.98 A	415 MW 2.986 275 MW 3.01 088 DT 2.95 115 DR 3.00 050 DT 2.91	221, 037
CHNO	Hydrogen isocyanate.....	(1.6) Q	246 MW 1.592 ^b	248
CHNS	Hydrogen isothiocyanate.....	(1.7) Q	207 MW 1.72 ^b	
CHP	Methylidyne phosphide (methinophosphide)	0.390 A	547 MW 0.390	
CH ₂ Br ₂	Dibromomethane.....	1.43 B	153 DT 1.43 271 DT 1.43	022
CH ₂ ClF	Chlorofluoromethane.....	1.82 B	344 DT 1.82	

^a In excited vibrational state 010.

^b Component along *a* axis.

7.2. Selected dipole moments (compounds containing carbon)–Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
CH ₂ ClNO ₂	Chloronitromethane.....	2.91 B	157 DR 2.91	112, 022, 012
CH ₂ Cl ₂	Dichloromethane.....	1.60 B	266 MW 1.63 153 DT 1.57 113 DT 1.54	
CH ₂ F ₂	Difluoromethane.....	1.97 A	262 MW 1.97	
CH ₂ N ₂	Cyanogen amide (cyanamide).....	4.27 C	413 MW 4.3 494 MW 4.24 ^a	
CH ₂ N ₂	Diazomethane.....	1.50 A	493a MW 1.50	377
CH ₂ N ₂	Diazirine.....	1.59 C	490 MW 1.59	534, 184, 584 ^b
CH ₂ O	Methanal (formaldehyde).....	2.33 A	246 MW 2.34 428 MW 2.33 237 MW 2.31 160 DR 2.29	
CH ₂ O ₂	Methanoic acid (formic acid).....	1.41 A	480 MW 1.415 ^c 058 DR 1.52 130 DR 1.4	
CH ₃ BF ₂	Methyl difluoroborane.....	1.66 B	364 MW 1.67 342 DT 1.62	
CH ₃ BO	Carbonyl borane.....	1.80 B	198 MW 1.795 ^c	100, 042, 566
CH ₃ Br	Bromomethane.....	1.81 A	219 MW 1.81 089 DT 1.80 113 DR 1.81 271 DT 1.83 118 DT 1.76	
CH ₃ Cl	Chloromethane.....	1.87 A	193 MW 1.87 219 MW 1.88 113 DR 1.89 038 DT 1.87 062 DT 1.87	
CH ₃ F	Fluoromethane.....	1.85 A	511 MW 1.8555 113 DT 1.85 089 DT 1.81 587 MW 1.8471	
CH ₃ F ₃ Ge	Methyl trifluorogermane.....	x Q	424 MW 3.8	

^a For ¹²C²H₂¹⁴N₂.

^b $\mu = 1.56 \pm 0.07$ D in the excited ¹A₂ electronic state.

^c For ¹²C¹H₃¹⁰B¹⁶O.

7.2. Selected dipole moments (compounds containing carbon) – Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
CH ₃ I	Iodomethane.....	1.62 B	321 DT 1.64 113 DR 1.62 089 DT 1.60 219 MW 1.65 118 DR 1.67	100, 042, 021
CH ₃ NO	Hydroxyliminomethane (formaldoxime).	0.44 A	484 MW 0.44 ↗ 491 MW 0.46 ↗	
CH ₃ NO	Formyl amide (formamide).....	3.73 B	351 MW 3.73 ↗ 064 DR 3.25	
CH ₃ NOS	Methyl sulfmlyamine.....	1.70 B	572 MW 1.70	
CH ₃ NO ₂	Nitritomethane (methyl nitrite).....	i	507 DR (a)	
CH ₃ NO ₂	Nitromethane.....	3.46 A	340 MW 3.48 298 DT 3.43 088 DT 3.44 118 DR 3.57	
CH ₃ NO ₃	Methyl nitrate.....	3.12 B	448 MW 3.12	
CH ₃ N ₃	Methyl azide.....	2.17 B	589 MW 2.17	
CH ₄	Methane.....	0 S	094 DT 0	012, 078
CH ₄ F ₂ Si	Methyl difluorosilane.....	2.11 A	389 MW 2.11 ↗	
CH ₄ O	Methanol.....	1.70 A	140 DT 1.71 113 DT 1.70 098 DT 1.70 033 DT 1.70	141, 229, 280, 001, 172
CH ₄ S	Methanethiol (methyl mercaptan).....	1.52 C	427 MW 1.52 ↗	350, 245
CH ₃ FSi	Methyl monofluorosilane.....	1.71 A	387 MW 1.71 ↗	
CH ₅ N	Methyl amine.....	1.31 B	354 MW 1.33 ^b ↗ 170 DT 1.30 113 DT 1.26 119 DT 1.35 062 DT 1.24	263, 137, 052, 055, 047
CH ₃ P	Methyl phosphine.....	1.10 A	452 MW 1.10	
CH ₃ Ge	Methyl germane.....	0.643 A	401 MW 0.635 444 MW 0.644 587 MW 0.6425	372, 373, Iso
CH ₃ OSi	Methoxysilane.....	1.17 B	548 DT 1.17	
CH ₃ Si	Methyl silane.....	0.735 A	349 MW 0.73 214 MW 0.73 587 MW 0.7351	Iso

^a $\mu = 2.22$ D at 308 °K.

^b For ¹²C²H₃¹⁴N²N₂.

7.2. Selected dipole moments (compounds containing carbon)—Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
CH ₆ Sn	Methyl stannane.....	0.68 C	238 MW 0.68	
C ₂ ClF ₃	Chlorotrifluoroethylene.....	0.40 D	325 DT 0.38	
			344 DR 0.58	
			314 DT 0.40	
C ₂ ClF ₅	Chloropentafluoroethane.....	0.52 C	314 DT 0.52	133
C ₂ Cl ₂ F ₄	1,2-Dichlorotetrafluoroethane.....	(0.5) Qi	336 DT 0.53	133, 416
			344 DT 0.46	
C ₂ F ₃ N	Trifluorocyanomethane.....	1.33 D	499 DR 1.33	
C ₂ F ₆	Hexafluoroethane.....	0 S	133
C ₂ F ₆ O	Bis(trifluoromethyl) ether.....	0.54 D	314 DT 0.54	
C ₂ N ₂	Dicyanogen (cyanogen).....	0 S	115 DT 0	050
C ₂ N ₂ S	Dicyano sulfide.....	3.02 A	569 MW 3.04	
			527aMW 3.01	
C ₂ HBr	Bromoacetylene.....	≤ 0.10 D	129 DT 0.0 ^a	
C ₂ HCl	Chloroacetylene.....	0.44 A	204 MW 0.44	
			129 DT 0.45	
C ₂ HCl ₅	Pentachloroethane.....	0.92 C	201 DT 0.92	
C ₂ HF	Fluoroacetylene.....	0.73 C	523 MW 0.73	413, 440
C ₂ HF ₃	Trifluoroethylene.....	1.40 C	518 MW 1.40	
C ₂ HF ₃ O ₂	Trifluoroethanoic acid (trifluoroacetic acid).	2.28 D	233 DR 2.28	
C ₂ HF ₅	Pentafluoroethane.....	1.54 C	314 DT 1.54	
C ₂ H ₂	Acetylene.....	0 S	009 DT 0	540 ^b
			094 DT 0	
C ₂ H ₂ Cl ₂	1,1-Dichloroethylene.....	1.34 A	477 MW 1.34	
C ₂ H ₂ Cl ₂	<i>cis</i> -1,2-Dichloroethylene.....	1.90 B	153 DT 1.90	
C ₂ H ₂ Cl ₂ F ₂	1,1-Dichloro-2,2-difluoroethane.....	i	315 DR (c)	
C ₂ H ₂ Cl ₂ O	Chloroacetyl chloride.....	2.23 Ci	065 DT 2.23	
C ₂ H ₂ Cl ₃ F	1,1,2-Trichloro-2-fluoroethane.....	i	315 DR (d)	
C ₂ H ₂ Cl ₄	1,1,2,2-Tetrachloroethane.....	1.32 Ci	201 DT 1.32	
			104 DR 1.36	
C ₂ H ₂ FN	Fluorocyanomethane.....	3.43 C	474 MW 3.43 [↗]	
C ₂ H ₂ F ₂	1,1-Difluoroethylene.....	1.38 A	196 MW 1.366	Iso
			587 MW 1.385	
			445 DR 1.41	
C ₂ H ₂ F ₂	<i>cis</i> -1,2-Difluoroethylene.....	2.42 A	453 MW 2.42	

^a Although the structure is unsymmetric, the dipole moment appears to be virtually zero.

^b Observation of a microwave transition of ¹²C₂¹H²H indicates that the dipole moment of this unsymmetric isotopic species is on the order of 0.01 D.

^c $\mu = 1.34$ D at 334 °K; 1.47 D at 474 °K.

^d $\mu = 1.38$ D at 379 °K; 1.44 D at 512 °K.

7.2. Selected dipole moments (compounds containing carbon) – Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C ₂ H ₂ N ₂ O	1,2,5-Oxadiazole.....	3.38 A	573 MW 3.38	Vib
C ₂ H ₂ N ₂ O	1,3,4-Oxadiazole.....	3.04 B	582 MW 3.04	
C ₂ H ₂ N ₂ S	1,2,5-Thiadiazole.....	1.56 A	505 MW 1.565	
C ₂ H ₂ N ₂ S	1,3,4-Thiadiazole.....	3.29 B	468 MW 3.29	
C ₂ H ₂ O	Methylene carbonyl (ketene).....	1.42 B	261 MW 1.414 166 DR 1.45 227aDR 1.46	
C ₂ H ₃ Br	Bromoethylene.....	1.42 B	135 DT 1.42	
C ₂ H ₃ Cl	Chloroethylene.....	1.45 B	135 DT 1.45 426 MW 1.420 ^a	
C ₂ H ₃ ClF ₂	1-Chloro-1,1-difluoroethane.....	2.14 B	315 DT 2.14	133
C ₂ H ₃ ClO	Acetyl chloride.....	2.72 C	065 DT 2.72	
C ₂ H ₃ ClO ₂	Methyl chloroformate.....	i	138 DR ^(b)	
C ₂ H ₃ Cl ₃	1,1,1-Trichloroethane.....	1.78 B	153 DT 1.79 155 DR 1.77	
C ₂ H ₃ Cl ₃	1,1,2-Trichloroethane.....	i	315 DR ^(c)	195, 201
C ₂ H ₃ F	Fluoroethylene.....	1.43 A	456 MW 1.427 ↗	
C ₂ H ₃ FO	Acetyl fluoride.....	2.96 A	409 MW 2.96 ↗	
C ₂ H ₃ F ₃	1,1,1-Trifluoroethane.....	2.32 B	219 MW 2.33 257 MW 2.28 133 DR 2.35	
C ₂ H ₃ F ₃	1,1,2-Trifluoroethane.....	1.58 B	516 MW 1.58 ^d	541, ^e 515, ^e 517, ^e 488
C ₂ H ₃ I	Iodoethylene.....	1.30 D	135 DR 1.30	208
C ₂ H ₃ N	Cyanomethane (acetonitrile).....	3.92 A	275 MW 3.94 446 DR 3.90 118 DT 3.96 113 DR 3.84 592 MW 3.918	
C ₂ H ₃ N	Isocyanomethane.....	3.85 B	275 MW 3.85	
C ₂ H ₃ NO	Methyl isocyanate.....	(2.8) Q	504aMW 2.81 ^f	
C ₂ H ₃ NS	Methyl thiocyanate.....	(4.0) Q	568 MW 4.03 ^f	
C ₂ H ₄	Ethylene.....	0 S	009 DT 0 094 DT 0	

^a Component along *a* axis.

^b $\mu = 2.41$ D at 308 °K; 1.55 D at 481 °K.

^c $\mu = 1.41$ D at 363 °K; 1.48 D at 513 °K.

^d For the *gauche* rotational isomer, which belongs to point group C₁.

^e These references give measurements on different rotational isomers of several isotopic species.

^f Component along *a* axis.

7.2. Selected dipole moments (compounds containing carbon—Continued)

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C ₂ H ₄ BrCl	1-Bromo-2-chloroethane.....	i	063 DR (a)	059
C ₂ H ₄ Br ₂	1,2-Dibromoethane.....	i	063 DR (b) 151 DR (b)	
C ₂ H ₄ ClF	1-Chloro-2-fluoroethane, <i>gauche</i> conformation.	2.72 C	567aMW 2.72	
C ₂ H ₄ ClF	1-Chloro-2-fluoroethane.....	i	315 DR (c)	
C ₂ H ₄ ClNO ₂	1-Chloro-1-nitroethane.....	3.27 B	157 DT 3.27	
C ₂ H ₄ Cl ₂	1,1-Dichloroethane.....	2.06 B	153 DT 2.06	032
C ₂ H ₄ Cl ₂	1,2-Dichloroethane.....	i	057 DR (d) 158 DR (d) 151 DR (d)	032, 053, 059, 061
C ₂ H ₄ Cl ₂ O	Bis(chloromethyl) ether.....	i	312 DR (e)	
C ₂ H ₄ F ₂	1,1-Difluoroethane.....	2.27 B	429 MW 2.30 ↗ 233 DT 2.24	
C ₂ H ₄ Ge	Germyl acetylene.....	0.136 A	581 MW 0.136	
C ₂ H ₄ O	Oxirane (ethylene oxide).....	1.89 A	232 MW 1.89 026 DT 1.90 113 DR 1.91 346 DT 1.91	
C ₂ H ₄ O	Ethanal (acetaldehyde).....	2.69 B	348 MW 2.69 ↗ 160 DR 2.72 065 DR 2.72	
C ₂ H ₄ O ₂	Ethanoic acid (acetic acid).....	1.74 C	058 DR 1.74	049
C ₂ H ₄ O ₂	Methyl methanoate (methyl formate).	1.77 B	394 MW 1.77 ↗	
C ₂ H ₄ S	Thiirane (ethylene sulfide).....	1.85 A	232 MW 1.85	
C ₂ H ₄ Si	Silyl acetylene.....	0.316 A	514 MW 0.316	
C ₂ H ₅ Br	Bromoethane.....	2.03 A	118 DT 2.02 089 DT 2.03	042, 112, 100, 021
C ₂ H ₅ BrO	Bromomethoxymethane.....	2.05 Ci	312 DR 2.05 †	

^a $\mu = 1.16$ D at 339 °K; 1.35 D at 436 °K.

^b Reference 063 gives $\mu = 1.02$ D at 339 °K; 1.19 D at 436 °K; reference 151 gives $\mu = 0.91$ D at 339 °K; 1.19 D at 496 °K.

^c $\mu = 1.84$ D at 309 °K; 1.97 D at 506 °K.

^d Reference 057 gives $\mu = 1.19$ D at 305 °K; 1.63 D at 544 °K; reference 151 gives $\mu = 1.24$ at 308 °K; 1.60 D at 525 °K; reference 158 gives $\mu = 1.24$ D at 307 °K; 1.46 D at 412 °K.

^e $\mu = 1.78$ D at 296 °K; 1.92 D at 467 °K.

^f μ seems to be constant in the temperature range 301 °K to 412 °K.

7.2. Selected dipole moments (compounds containing carbon)—Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C ₂ H ₅ Cl	Chloroethane.....	2.05 A	371 MW 1.745 ^a 038 DT 2.06 062 DT 2.03 113 DR 2.07 175 DR 1.98	035, 308, 024, 042, 043, 100
C ₂ H ₅ ClO	2-Chloroethanol.....	1.78 Ci	064 DR 1.78	
C ₂ H ₅ ClO	Chloromethoxymethane.....	i	315 DR ^(b) 312 DR ^(b)	
C ₂ H ₅ F	Fluoroethane.....	1.94 B	320 MW 1.96 ↗ 089 DT 1.92	
C ₂ H ₅ I	Iodoethane.....	1.91 B	425 MW 1.77 ↗ 089 DT 1.92 118 DR 1.90	021, 042, 100, 112
C ₂ H ₅ N	Iminoethane (ethyleneimine).....	1.90 A	281 MW 1.90	
C ₂ H ₅ N	Methyliminomethane (CH ₃ N=CH ₂)...	1.53 B	545 MW 1.53	
C ₂ H ₅ NO	Acetyl amine (acetamide).....	3.76 Bi	539 DR 3.76	
C ₂ H ₅ NO	Methylaminomethanal (<i>N</i> -methylformamide).	3.83 Bi	539 DR 3.83	
C ₂ H ₅ NO ₂	Nitritoethane (ethyl nitrite).....	2.40 Ci	083 DR 2.38 313 DR 2.42	
C ₂ H ₅ NO ₂	Nitroethane.....	3.65 B	157 DR 3.69 118 DR 3.61	
C ₂ H ₆	Ethane.....	0 S	009 DT 0 094 DT 0	
C ₂ H ₆ AlCl	Dimethylaluminum chloride.....	x Q	154
C ₂ H ₆ BF	Dimethyl fluoroborane.....	1.32 C	342 DT 1.32	
C ₂ H ₆ O	Ethanol.....	1.69 Bi	033 DR 1.69 060 DT 1.70 098 DT 1.68	509, 014, 411 140
C ₂ H ₆ O	Dimethyl ether.....	1.30 A	503 MW 1.302 026 DT 1.30 062 DT 1.30 113 DT 1.29 119 DT 1.31 561 DT 1.29	034, 043

^a Component along *a* axis.

^b Reference 315 gives $\mu=2.03$ D at 347 °K; 2.07 D at 507 °K; reference 312 gives $\mu=1.77$ D at 296 °K; 1.92 D at 467 °K.

7.2. Selected dipole moments (compounds containing carbon) – Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C ₂ H ₆ OS	Dimethylsulfoxide.....	3.96 A	532aMW 3.96 ↗	
C ₂ H ₆ O ₂	1,2-Ethanediol (ethylene glycol).....	2.28 Ci	064 DR 2.28	
C ₂ H ₆ O ₂ S	Dimethyl sulfoxylate (dimethyl sulfone).	4.49 B	143 DR 4.49	
C ₂ H ₆ S	Ethanethiol.....	1.58 Bi	108 DT 1.58	
C ₂ H ₆ S	Dimethyl sulfide.....	1.50 A	459 MW 1.50	
C ₂ H ₆ Si	Silyl ethylene.....	0.66 A	457 MW 0.662	
C ₂ H ₇ B ₅	2,4-Dicarbaborane.....	1.32 B	550 MW 1.32	
C ₂ H ₇ N	Aminoethane (ethyl amine).....	1.22 Ci	206 DT 1.22	052
C ₂ H ₇ N	Dimethyl amine.....	1.03 B	170 DT 1.03 119 DT 1.03 062 DT 0.97	137, 055, 052, 047
C ₂ H ₇ P	Ethyl phosphine.....	1.17 Bi	352 DT 1.17	
C ₂ H ₇ P	Dimethyl phosphine.....	1.23 A	519 MW 1.23	
C ₂ H ₈ N ₂	1,2-Diaminoethane.....	1.99 Ci	064 DR 1.99	
C ₂ H ₈ Si	Dimethyl silane.....	0.75 A	458 MW 0.75	
C ₂ H ₈ Si	Ethyl silane.....	0.81 B	436 MW 0.81	
C ₃ Cl ₃ F ₃	1,1,2-Trichloro-3,3,3-trifluoropropene.	1.28 D	273 DR 1.28	
C ₃ O ₂	Dicarbonyl carbon (carbon suboxide).	0 S	352 DT 0	
C ₃ HF ₃	3,3,3-Trifluoropropyne.....	2.36 B	247 MW 2.36	
C ₃ HF ₇	1,1,2,2,3,3,3-Heptafluoropropane.....	1.62 Di	325 DT 1.62	
C ₃ HN	Cyanoacetylene.....	3.72 A	226 MW 3.6 593 MW 3.724	
C ₃ H ₂ N ₂	Dicyanomethane.....	3.73 A	422 MW 3.735	
C ₃ H ₂ O	Propynal.....	2.47 B	319 MW 2.47 ↗	585 ^a
C ₃ H ₂ O ₃	Vinylene carbonate.....	4.55 A	304 MW 4.53 583 MW 4.57	
C ₃ H ₃ Br	3-Bromopropyne.....	1.54 C	345 DR 1.54	
C ₃ H ₃ Cl	3-Chloropropyne.....	1.68 C	449 MW 1.68 ↗ 345 DR 1.67	381
C ₃ H ₃ F ₃	3,3,3-Trifluoropropene.....	2.45 B	273 DR 2.45	
C ₃ H ₃ N	Cyanoethylene.....	3.87 B	307 MW 3.91 ↗ 160 DT 3.83	
C ₃ H ₃ NO	Acetyl cyanide.....	3.45 B	400 MW 3.45 ↗	
C ₃ H ₃ NS	Thiazole.....	1.62 B	467 MW 1.62	
C ₃ H ₄	Cyclopropene.....	0.45 A	398 MW 0.454	
C ₃ H ₄	Propyne.....	0.781 A	136 DR 0.78 115 DT 0.72 275 MW 0.75 587 MW 0.781	257, Iso

^a In the excited 'A' electronic state, the *a* component of the moment is 0.7 ± 0.2 D.

7.2. Selected dipole moments (compounds containing carbon)—Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C ₃ H ₄	Propadiene (allene).....	0 S	115 DT 0	
C ₃ H ₄ Cl ₂	1,1-Dichlorocyclopropane.....	1.58 B	473 MW 1.58	
C ₃ H ₄ Cl ₂	1,3-Dichloropropene, bp 104 °C isomer.	i	195 DR 1.79	
C ₃ H ₄ Cl ₂	1,3-Dichloropropene, bp 112 °C isomer.	i	195 DR 1.81	
C ₃ H ₄ Cl ₂	2,3-Dichloropropene.....	i	195 DR (a)	
C ₃ H ₄ Cl ₂ O	1,1-Dichloropropanone.....	i	311 DR (b)	
C ₃ H ₄ Cl ₄	1,1,2,2-Tetrachloropropane.....	i	362 DR (c)	302
C ₃ H ₄ O	Ethylidene carbonyl (methyl ketene)...	1.79 B	590 MW 1.79 ↗	469
C ₃ H ₄ O	Propenal, <i>trans</i> conformation (acrolein).	3.12 B	370 MW 3.12 ↗ 166 DR 3.04 ^d	
C ₃ H ₄ O ₂	2-Oxoöxetane (β -propiolactone).....	4.18 A	333 MW 4.20 ↗ 551 MW 4.17	
C ₃ H ₄ O ₂	Vinyl formate.....	1.49 A	544 MW 1.49 ↗	
C ₃ H ₅ Br	3-Bromopropene.....	(1.9) Q	020 DR 1.93	
C ₃ H ₅ Cl	2-Chloropropene.....	1.66 B	165 DT 1.66 020 DR 1.66	
C ₃ H ₅ Cl	<i>cis</i> -1-Chloropropene.....	1.67 C	529 MW 1.64 ↗ 165 DR 1.71	
C ₃ H ₅ Cl	<i>trans</i> -1-Chloropropene.....	1.97 C	165 DR 1.97	
C ₃ H ₅ Cl	3-Chloropropene.....	1.94 Ci	121 DT 1.90 165 DR 1.98	100, 042
C ₃ H ₅ ClO	Chloropropanone.....	i	065 DR (e)	
C ₃ H ₅ ClO ₂	Ethyl chloroformate.....	i	138 DR (f)	
C ₃ H ₅ Cl ₃	1,2,2-Trichloropropane.....	i	362 DR (g)	303
C ₃ H ₅ F	<i>cis</i> -1-Fluoropropene.....	1.46 B	470 MW 1.46 ↗	
C ₃ H ₅ F	<i>trans</i> -1-Fluoropropene.....	(1.9) Q	365 MW 1.86 ^h	
C ₃ H ₅ F	2-Fluoropropene.....	1.61 B	410 MW 1.61 ↗	
C ₃ H ₅ F	3-Fluoropropene, <i>cis</i> conformation....	1.76 A	560 MW 1.765 ↗	
C ₃ H ₅ F	3-Fluoropropene, <i>gauche</i> conformation.	1.94 A	560 MW 1.939 ↗	

^a $\mu = 1.74$ D at 397 °K; 1.77 D at 518 °K.

^b $\mu = 1.93$ D at 338 °K; 2.07 D at 468 °K.

^c $\mu = 1.56$ D at 372 °K; 1.59 D at 467 °K.

^d There was no apparent change in the average value of the dipole moment over the temperature range 377 to 478 °K. Although other conformations are possible, the microwave spectrum indicates that the *trans* conformation is predominant at room temperature.

^e $\mu = 2.21$ D at 336 °K; 2.29 D at 454 °K.

^f $\mu = 1.57$ D at 308 °K; 1.47 D at 480 °K.

^g $\mu = 1.63$ D at 354 °K; 1.67 D at 468 °K.

^h Component along *a* axis.

7.2. Selected dipole moments (compounds containing carbon)—Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C ₃ H ₅ N	Cyanoethane (propionitrile).....	4.02 A	402 MW 4.02 ↗ 118 DT 4.05 160 DR 4.00	
C ₃ H ₅ NO ₂	3-Nititropene (allyl nitrite).....	i	507 DR (a)	
C ₃ H ₆	Cyclopropane.....	0 S	113 DT 0	
C ₃ H ₆	Propene.....	0.366 A	356 MW 0.366 ↗ 074 DT 0.35 094 DT 0.34	
C ₃ H ₆ Br ₂	1,2-Dibromopropane.....	i	362 DR (b)	303
C ₃ H ₆ ClNO ₂	1-Chloro-1-nitropropane.....	3.48 Bi	157 DT 3.48	
C ₃ H ₆ Cl ₂	1,2-Dichloropropane.....	i	195 DR (c)	
C ₃ H ₆ Cl ₂	1,3-Dichloropropane.....	2.08 Bi	104 DT 2.08 ^d	
C ₃ H ₆ Cl ₂	2,2-Dichloropropane.....	2.27 C	153 DR 2.27	
C ₃ H ₆ O	Oxetane (trimethylene oxide).....	1.94 A	418 MW 1.94 346 DT 1.94	317
C ₃ H ₆ O	Methyl oxirane (propylene oxide).....	2.01 A	367 MW 2.01 ↗	
C ₃ H ₆ O	Propanone (acetone).....	2.88 A	412 MW 2.90 344 DT 2.88 272 DT 2.89 026 DT 2.87 113 DR 2.87 065 DR 2.88	112
C ₃ H ₆ O	2-Propen-1-ol (allyl alcohol).....	1.60 C	099 DT 1.60	
C ₃ H ₆ O	Propanal, <i>cis</i> conformation (propionaldehyde).	2.52 B	531 MW 2.52 ↗ 160 DT 2.72 ^e	
C ₃ H ₆ O ₂	Propanoic acid.....	1.75 Ci	058 DR 1.75	
C ₃ H ₆ O ₂	Methyl acetate.....	1.72 Ci	138 DT 1.72 066 DR 1.72	
C ₃ H ₆ O ₂	Ethyl formate.....	1.93 Ci	066 DT 1.93	
C ₃ H ₆ O ₃	Dimethyl carbonate.....	i	122 DR (f)	
C ₃ H ₆ O ₃	1,3,5-Trioxane.....	2.08 A	542 MW 2.07 227 MW 2.09	

^a $\mu = 2.25$ D at 298 °K.

^b $\mu = 1.17$ D at 354 °K; 1.41 D at 467 °K.

^c $\mu = 1.46$ D at 345 °K; 1.68 D at 506 °K.

^d The value of the dipole moment appears to be constant over the temperature range 374 to 485 °K.

^e Equilibrium mixture of conformations in which the average dipole moment is essentially constant over the temperature range 354 to 508 °K.

^f $\mu = 0.90$ D at 328 °K; 1.05 D at 479 °K.

7.2. Selected dipole moments (compounds containing carbon)–Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C ₃ H ₆ S	Thietane (trimethylene sulfide).....	1.85 C	577 MW 1.85	
C ₃ H ₆ S	Methyl thiirane (propylene sulfide)....	1.95 A	504 MW 1.95	
C ₃ H ₇ Br	1-Bromopropane.....	2.18 Ci	118 DR 2.18	100, 042
C ₃ H ₇ Br	2-Bromopropane.....	2.21 C	118 DR 2.21	
C ₃ H ₇ Cl	1-Chloropropane.....	2.05 Bi	062 DT 2.05	112, 100, 043, 042, 053, 035
C ₃ H ₇ Cl	2-Chloropropane.....	2.17 C	118 DR 2.17	
C ₃ H ₇ F	1-Fluoropropane, <i>gauche</i> conformation.	1.90 C	476 MW 1.90 ↗	
C ₃ H ₇ F	1-Fluoropropane, <i>trans</i> conformation.	2.05 B	476 MW 2.05 ↗	
C ₃ H ₇ I	1-Iodopropane.....	2.04 Ci	118 DR 2.04	100, 042
C ₃ H ₇ N	3-Aminopropane.....	(1.2) Q	020 DR 1.20	
C ₃ H ₇ NO	N,N-Dimethylformamide.....	3.82 Bi	539 DR 3.82	
C ₃ H ₇ NO	Acetyl methylamine (<i>N</i> -Methylacetamide).	3.73 Bi	539 DR 3.73	
C ₃ H ₇ NO ₂	1-Nitritopropane (<i>n</i> -propyl nitrite).....	i	507 DR (a)	
C ₃ H ₇ NO ₂	2-Nitritopropane (isopropyl nitrite).....	i	313 DR (b)	
C ₃ H ₇ NO ₂	1-Nitropropane.....	3.66 Bi	118 DR 3.60 155 DR 3.72	
C ₃ H ₇ NO ₂	2-Nitropropane.....	3.73 B	155 DR 3.73	
C ₃ H ₈	Propane.....	0.084 A	431 MW 0.083 587 MW 0.085	352, 277, 094, 074, Iso
C ₃ H ₈ O	1-Propanol.....	1.68 Bi	033 DT 1.69 099 DT 1.67	
C ₃ H ₈ O	2-Propanol.....	1.66 Bi	098 DT 1.60 127 DT 1.69	
C ₃ H ₈ O	Methoxyethane (methyl ethyl ether)...	1.23 Ci	194 DT 1.23	
C ₃ H ₈ O ₂	Dimethoxymethane.....	i	109 DR (c)	
C ₃ H ₉ Al	Trimethyl aluminum.....	x Q	154
C ₃ H ₉ As	Trimethyl arsine.....	0.86 B	404 MW 0.86	
C ₃ H ₉ BF ₃ N	Trimethyl aminc – boron trifluoride complex.	(5) Q	438 MW 5	
C ₃ H ₉ N	Trimethyl amine.....	0.612 A	383 MW 0.612 423 NR 0.61 343 NR 0.60 170 DT 0.65 119 DT 0.67 062 DT 0.61	137, 055, 052, 047
C ₃ H ₉ N	1-Aminopropane (<i>n</i> -propylamine).....	1.17 Ci	228 DT 1.17	020

^a $\mu = 2.42$ D at 298 °K.

^b $\mu = 2.58$ D from 256 to 332 °K.

^c $\mu = 0.77$ D at 307 °K; 1.17 D at 482 °K.

7.2. Selected dipole moments (compounds containing carbon)—Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C ₃ H ₉ P	Trimethyl phosphine.....	1.19 A	384 MW 1.192	
C ₃ H ₁₀ Si	Trimethyl silane.....	0.525 A	437 MW 0.525	
C ₄ Cl ₃ F ₇	2,2,3-Trichloroheptafluorobutane.....	(0.9) Qi	336 DT 0.85	
C ₄ F ₈	Perfluorocyclobutane.....	0 S	314 DT 0	
C ₄ F ₈ O	Perfluoroöxolane (perfluorotetra- methylene oxide).	0.56 D	325 DT 0.56	
C ₄ F ₁₀ O	Perfluoro(ethoxyethane).....	0.47 Di	325 DT 0.51 314 DT 0.42	
C ₄ H ₂ N ₂	<i>trans</i> -1,2-Dicyanoethylene.....	0 S	151
C ₄ H ₄	1-Buten-3-yne.....	(0.4) Q	496 MW 0.43 ^a	
C ₄ H ₄ Cl ₂	1,4-Dichloro-2-butyne.....	2.10 Bi	363 DR 2.10	
C ₄ H ₄ F ₂	1,1-Difluoro-1,3-butadiene (<i>trans</i> conformation).	1.29 A	549 MW 1.29	
C ₄ H ₄ N ₂	1,2-Dicyanoethane.....	i	151 DR (b)	
C ₄ H ₄ O	Furan.....	0.66 A	249 MW 0.664 278 DT 0.72	
C ₄ H ₄ O	3-Butyne-2-one.....	(2.4) Q	521 MW 2.4	
C ₄ H ₄ O ₂	Diketene.....	3.53 B	160 DR 3.53	
C ₄ H ₄ S	Thiophene.....	0.55 C	278 DT 0.55 108 DT 0.56	
C ₄ H ₅ Cl	4-Chloro-1,2-butadiene.....	2.02 Ci	165 DR 2.02	
C ₄ H ₅ Cl	1-Chloro-2-butyne.....	2.19 C	345 DR 2.19	
C ₄ H ₅ F	2-Fluoro-1,3-butadiene (<i>trans</i> conformation).	1.42 A	486 MW 1.417 ↗	
C ₄ H ₅ N	Pyrrrole.....	1.84 C	270 DT 1.84	327
C ₄ H ₅ N	<i>cis</i> -1-Cyanopropene.....	4.08 B	502 MW 4.08 ↗	
C ₄ H ₅ N	<i>trans</i> -1-Cyanopropene.....	4.50 B	160 DR 4.50	
C ₄ H ₅ N	2-Cyanopropene (methacrylonitrile)...	3.69 C	166 DR 3.69	
C ₄ H ₆	Cyclobutene.....	0.132 A	563 MW 0.132	
C ₄ H ₆	1-Butyne.....	0.80 C	136 DR 0.80	
C ₄ H ₆	1,2-Butadiene.....	0.403 A	357 MW 0.403 ↗	
C ₄ H ₆	1,3-Butadiene.....	0 S	159 DT 0 ^c	

^a Component along *a* axis.

^b $\mu = 3.47$ D at 443 °K; 3.59 D at 513 °K.

^c Although unsymmetric conformations may exist, the *trans* conformation predominates at normal temperatures.

7.2. Selected dipole moments (compounds containing carbon)–Continued

Formula	Compound name	Selected moment (dcbyes)	Basic references	Other data
C ₄ H ₆ O	Cyclobutanone.....	2.99 B	500aMW 2.99	063
C ₄ H ₆ O	<i>trans</i> -2-Butenal (crotonaldehyde).....	3.67 Bi	160 DR 3.67	
C ₄ H ₆ O	2-Methylpropenal (methacrolein).....	2.68 Ci	166 DR 2.68	
C ₄ H ₆ O	3-Butene-2-one.....	3.16 B	557 MW 3.16 ↗	
C ₄ H ₆ O ₂	2,3-Butanedione.....	(0) Qi	151 DT (a)	
C ₄ H ₆ O ₃	Acetyl acetate (acetic anhydride).....	(2.8) Qi	082 DR 2.8	
C ₄ H ₆ S	Divinyl sulfide.....	1.20 D	165 DR 1.20	
C ₄ H ₇ Cl	1-Chloro-2-methylpropene.....	1.95 Bi	160 DT 1.95 165 DR 1.85	
C ₄ H ₇ Cl ₃	1,1,2-Trichloro-2-methylpropane.....	1.86 Ci	362 DR 1.86	
C ₄ H ₇ F	Fluorocyclobutane.....	1.94 A	586 MW 1.94	
C ₄ H ₇ N	1-Cyanopropane.....	4.07 Bi	118 DR 4.07	
C ₄ H ₈	1-Butene.....	0.34 Ci	009 DT 0.38 115 DT 0.30	
C ₄ H ₈	<i>cis</i> -2-Butene.....	0.3 D	344 DT 0.33	
C ₄ H ₈	<i>trans</i> -2-Butene.....	0 S	115 DT 0	
C ₄ H ₈	2-Methylpropene.....	0.50 A	454 MW 0.503 115 DT 0.49	
C ₄ H ₈ Br ₂	1,2-Dibromo-2-methylpropane.....	i	362 DR (b)	303
C ₄ H ₈ Cl ₂	1,4-Dichlorobutane.....	2.22 Ci	195 DR 2.22	
C ₄ H ₈ Cl ₂	1,2-Dichloro-2-methylpropane.....	i	362 DR (c)	
C ₄ H ₈ O	Tetrahydrofuran.....	1.63 C	346 DT 1.63	
C ₄ H ₈ O	<i>cis</i> -2,3-Dimethyloxirane.....	2.03 A	464 MW 2.03 ↗	
C ₄ H ₈ O	Butanal.....	2.72 Bi	160 DR 2.72	
C ₄ H ₈ O ₂	1,4-Dioxane.....	0 S	111 DT 0 087 DT 0	
C ₄ H ₈ O ₂	Ethyl acetate.....	1.78 Ci	066 DT 1.78	
C ₄ H ₉ Br	1-Bromobutane.....	2.08 Ci	118 DT 2.08	
C ₄ H ₉ Br	2-Bromobutane.....	2.23 Ci	118 DR 2.23	
C ₄ H ₉ Cl	1-Chlorobutane.....	2.05 Bi	105 DT 2.05 118 DR 2.14	
C ₄ H ₉ Cl	2-Chlorobutane.....	2.04 Ci	155 DT 2.04	

^a Although unsymmetric *gauche* conformations are possible, the polarization shows no dependence on temperature and is consistent with the *trans* conformation. This interpretation, however, implies an exceptionally large vibrational polarization.

^b $\mu = 1.20$ D at 354 °K; 1.27 D at 412 °K.

^c $\mu = 1.56$ D at 339 °K; 1.66 D at 467 °K.

7.2. Selected dipole moments (compounds containing carbon)—Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C ₄ H ₉ Cl	1-Chloro-2-methylpropane.....	2.00 Ci	155 DT 2.00	269
C ₄ H ₉ Cl	2-Chloro-2-methylpropane.....	2.13 B	155 DR 2.13	
C ₄ H ₉ F	2-Fluoro-2-methylpropane.....	1.96 A	384 MW 1.959	
C ₄ H ₉ I	1-Iodobutane.....	2.12 Ci	118 DR 2.12	
C ₄ H ₉ NO	Propanoyl methylamine (N-methylpropionamide).	3.61 Bi	539 DR 3.61	
C ₄ H ₉ NO	Acetyl dimethylamine (N,N-dimethylacetamide).	3.81 Bi	539 DR 3.81	
C ₄ H ₉ NO ₂	2-Nitrito-2-methylpropane (t-butyl nitrite).	2.74 Ci	508 DR 2.77 313 DR 2.71	
C ₄ H ₉ NO ₂	1-Nitrobutane.....	3.59 Bi	118 DR 3.59	
C ₄ H ₉ NO ₂	2-Nitro-2-methylpropane.....	3.71 B	155 DR 3.71	
C ₄ H ₁₀	Butane.....	≤ 0.05 Ci	277 DT ≤ 0.05	115
C ₄ H ₁₀	2-Methylpropane.....	0.132 A	384 MW 0.132 337 NR 0.132 277 DT 0.13	432, 115, Iso
C ₄ H ₁₀ O	1-Butanol.....	1.66 Bi	099 DT 1.65 033 DT 1.67	112
C ₄ H ₁₀ O	2-Methylpropan-1-ol (isobutanol).....	1.64 C	098 DT 1.64	146, 044, 038, 034, 014
C ₄ H ₁₀ O	Diethyl ether.....	1.15 Bi	194 DT 1.13 026 DT 1.15 062 DT 1.11 119 DT 1.19	
C ₄ H ₁₀ S	Diethyl sulfide.....	1.54 Ci	108 DT 1.54	
C ₄ H ₁₁ N	1-Aminobutane (n-butylamine).....	(1.0) Qi	228 DT 1.00 ^a	
C ₄ H ₁₁ N	Diethyl amine.....	0.92 Ci	206 DT 0.92	052
C ₅ F ₁₂	Perfluoropentane.....	≤ 0.10 Di	233 DT 0 ^b	
C ₅ F ₁₂	Perfluoro (2-methylbutane).....	≤ 0.10 Di	233 DT 0 ^b	
C ₅ H ₅ N	Pyridine.....	2.19 B	329 DT 2.23 289 MW 2.15	
C ₅ H ₅ N	1-Cyano-1,3-butadiene.....	3.90 Ci	166 DR 3.90	
C ₅ H ₆	1,3-Cyclopentadiene.....	0.419 A	164 DR 0.53 574 MW 0.419 334 MW 0.418	

^a The extrapolated value of polarization (vs 1/T) determined for this compound is inconsistent with the other aminoalkanes. The dipole moment given is probably low.

^b Although unsymmetric conformations are likely, the dipole moment appears to be virtually zero.

7.2. Selected dipole moments (compounds containing carbon)–Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C ₅ H ₈	Cyclopentene.....	0.20 B	555 MW 0.190 ^a 492 MW 0.22	
C ₅ H ₈	1-Pentyne.....	0.81 Ci	136 DR 0.86 559 DR 0.81 ^b	
C ₅ H ₈	<i>trans</i> -1,3-Pentadiene.....	0.68 Di	159 DR 0.68	
C ₅ H ₈	2-Methyl-1,3-butadiene (<i>trans</i> conformation).	0.25 A	538 MW 0.25 ^γ	159
C ₅ H ₈ Br ₄	1,3-Dibromo-2,2-bis(bromomethyl) propane.	x Q	068
C ₅ H ₈ O	Cyclopentanone.....	(3.3) Q	399 MW 3.30 ^c	
C ₅ H ₈ O ₂	Acetylacetone.....	Ci	082 DR 3.05 ^d	
C ₅ H ₉ N	1-Cyanobutane.....	4.12 Bi	097 DT 4.12	
C ₅ H ₉ N	2-Cyano-2-methylpropane.....	3.95 A	489 MW 3.95	
C ₅ H ₁₀	Ethylcyclopropane.....	(0.5) Q	020 DR 0.47	
C ₅ H ₁₀	1-Pentene.....	(0.5) Q	020 DR 0.51	
C ₅ H ₁₀ O ₃	Diethyl carbonate.....	1.10 Ci	110 DT 1.10	
C ₅ H ₁₁ Br	1-Bromopentane.....	2.20 Ci	314 DR 2.20	
C ₅ H ₁₁ Cl	1-Chloropentane.....	2.16 Ci	118 DR 2.16	
C ₅ H ₁₂	Pentane.....	< 0.1 Di	277 DT < 0.07 352 DT < 0.05	098, 020, 112
C ₅ H ₁₂	2-Methylbutane.....	0.13 C	352 DT 0.13 277 DT 0.1	
C ₅ H ₁₂	2,2-Dimethylpropane.....	0 S	277 DT 0	
C ₅ H ₁₂ O ₂	Diethoxymethane.....	i	110 DR (e)	
C ₅ H ₁₂ O ₄	Tetramethoxymethane.....	0 Qi	038 DT ≈ 0	030
C ₆ H ₂ Cl ₂ O ₂	2,5-Dichloro-1,4-cyclohexadienedione..	0 S	131 DT 0	
C ₆ H ₄ BrF	<i>p</i> -Bromofluorobenzene.....	(0.5) Q	156 DR 0.5	
C ₆ H ₄ ClNO ₂	<i>o</i> -Chloronitrobenzene.....	4.64 B	120 DR 4.64	
C ₆ H ₄ ClNO ₂	<i>m</i> -Chloronitrobenzene.....	3.73 B	120 DR 3.73	
C ₆ H ₄ ClNO ₂	<i>p</i> -Chloronitrobenzene.....	2.83 B	120 DR 2.83	
C ₆ H ₄ Cl ₂	<i>o</i> -Dichlorobenzene.....	2.50 B	194 DR 2.48 156 DT 2.52	120
C ₆ H ₄ Cl ₂	<i>m</i> -Dichlorobenzene.....	1.72 C	120 DR 1.72	
C ₆ H ₄ Cl ₂	<i>p</i> -Dichlorobenzene.....	0 S	120 DR 0	
C ₆ H ₄ FI	<i>p</i> -Iodofluorobenzene.....	0.89 D	156 DR 0.89	
C ₆ H ₄ FNO ₂	<i>p</i> -Fluoronitrobenzene.....	2.87 B	156 DR 2.87	
C ₆ H ₄ F ₂	<i>m</i> -Difluorobenzene.....	1.58 B	194 DT 1.58	

^a Component along *b* axis. The component along *c* axis was estimated to be 0.05 to 0.10 D.

^b Allowance for vibrational polarization has been made. See reference 559.

^c Component along *a* axis.

^d Mixture of enol and keto forms.

^e $\mu = 1.26$ D at 329 °K; 1.32 D at 476 °K.

7.2. Selected dipole moments (compounds containing carbon)—Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data	
C ₆ H ₄ N ₂ O ₄	<i>p</i> -Dinitrobenzene.....	0 S	131 DT 0	068	
C ₆ H ₄ O ₂	1,4-Cyclohexadienedione (<i>p</i> -benzoquinone).	0 S	131 DT 0		
C ₆ H ₅ Br	Bromobenzene.....	1.70 B	097 DT 1.70 321 DT 1.70 156 DR 1.77	156, 273, 539	
C ₆ H ₅ Cl	Chlorobenzene.....	1.69 B	101 DT 1.71 084 DT 1.70 194 DT 1.67 520 MW 1.78		
C ₆ H ₅ ClO	<i>o</i> -Chlorophenol.....	i	148 DR (a)		
C ₆ H ₅ ClO	<i>p</i> -Chlorophenol.....	2.11 C	148 DR 2.11		
C ₆ H ₅ F	Fluorobenzene.....	1.60 C	101 DT 1.58 194 DR 1.60 395 MW 1.66		
C ₆ H ₅ I	Iodobenzene.....	1.70 C	156 DR 1.70 321 DT 1.71		
C ₆ H ₅ NO ₂	Nitrobenzene.....	4.22 B	101 DT 4.22 084 DR 4.27		
C ₆ H ₆	Benzene.....	0 S	084 DT 0 113 DT 0 074 DT 0		157, 112, 011, 336
C ₆ H ₆ N ₂ O ₂	<i>p</i> -Aminonitrobenzene (<i>p</i> -nitroaniline)..	x Q		068, 080
C ₆ H ₆ O	Phenol.....	1.45 C	120 DR 1.45		068
C ₆ H ₆ O ₂	<i>p</i> -Dihydroxybenzene.....	x Q		
C ₆ H ₇ N	Aminobenzene (aniline).....	1.53 C	120 DR 1.53		
C ₆ H ₈	1,3-Cyclohexadiene.....	0.44 B	553 MW 0.437		
C ₆ H ₈	1,5-Hexadiyne.....	i	559 DR 0.57 ^{b,c}		
C ₆ H ₈ N ₂	<i>o</i> -Diaminobenzene.....	1.53 Di	148 DR 1.53		
C ₆ H ₈ N ₂	<i>m</i> -Diaminobenzene.....	1.81 Di	148 DR 1.81		
C ₆ H ₈ N ₂	<i>p</i> -Diaminobenzene.....	1.53 Di	148 DR 1.53		
C ₆ H ₈ O ₂	1,4-Cyclohexanedione.....	(1.4) Qi	463 DR 1.41		
C ₆ H ₁₀	Cyclohexene.....	0.55 D	121 DR 0.55		
C ₆ H ₁₀	1-Hexyne.....	0.83 Ci	559 DR 0.83 ^b 136 DR 0.89		

^a $\mu = 1.24$ D at 421 °K; 1.37 D at 562 °K.

^b An allowance has been made for vibrational polarization. See reference 559.

^c At 308 °K.

7.2. Selected dipole moments (compounds containing carbon)–Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C ₆ H ₁₀	2-Methyl-1,3-pentadiene.....	0.65 D	164 DR 0.65	
C ₆ H ₁₀	3-Methyl-1,3-pentadiene.....	0.63 Di	164 DR 0.63	
C ₆ H ₁₀	3,3-Dimethyl-1-butyne.....	0.66 A	489 MW 0.661	
C ₆ H ₁₀	2-Ethyl-1,3-butadiene.....	(0.45) Qi	164 DR 0.45	
C ₆ H ₁₀	2,3-Dimethyl-1,3-butadiene.....	0.52 Di	159 DR 0.52	
C ₆ H ₁₀ BrCl	<i>trans</i> -1-Bromo-2-chlorocyclohexane.....	i	463 DR 2.19 ^a	
C ₆ H ₁₀ Br ₂	<i>trans</i> -1,2-Dibromocyclohexane.....	i	463 DR 2.00 ^a	
C ₆ H ₁₀ Cl ₂	<i>cis</i> -1e,2a-Dichlorocyclohexane.....	3.11 C	287 DR 3.11	
C ₆ H ₁₀ Cl ₂	<i>trans</i> -1,2-Dichlorocyclohexane.....	i	287 DR 2.31 ^a 463 DR 2.29 ^a	
C ₆ H ₁₀ O ₃	Ethyl acetoacetate.....	i	082 DR 2.98 ^b	
C ₆ H ₁₂ N ₂	Diisopropylidene hydrazine (dimethyl ketazine).	1.53 Bi	151 DT 1.53	
C ₆ H ₁₂ O ₂	Pentyl formate (n-amyl formate).....	1.90 Ci	066 DT 1.90	
C ₆ H ₁₂ O ₃	2,4,6-Trimethyl-1,3,5-trioxane (paraldehyde).	1.43 C	212 DT 1.43	
C ₆ H ₁₄	Hexane.....	≤ 0.1 Di	090 DT ≈ 0 098 DR ≈ 0	
C ₆ H ₁₄ O	Dipropyl ether.....	1.21 Ci	119 DT 1.21 062 DR 1.30	034
C ₆ H ₁₄ O	Diisopropyl ether.....	1.13 Di	251 DT 1.13	
C ₆ H ₁₄ O ₂	1,1-Diethoxyethane.....	i	110 DR (c)	
C ₆ H ₁₅ N	Triethyl amine.....	0.66 Ci	206 DT 0.66	052
C ₆ H ₁₈ OSi ₂	Bis(trimethylsilyl) ether.....	(0.66) Qi	318 DR 0.66	
C ₇ H ₄ ClF ₃	<i>o</i> -Chloro(trifluoromethyl)benzene.....	3.46 B	273 DR 3.46	
C ₇ H ₄ ClF ₃	<i>p</i> -Chloro(trifluoromethyl)benzene.....	1.58 C	273 DR 1.58	
C ₇ H ₄ N ₂ O ₂	<i>p</i> -Cyanonitrobenzene.....	(0) Q	131 DT ≈ 0	
C ₇ H ₅ F ₃	(Trifluoromethyl)benzene.....	2.86 B	273 DR 2.86	
C ₇ H ₅ N	Cyanobenzene (benzonitrile).....	4.18 B	299 MW 4.18 ^d 084 DR 4.42	
C ₇ H ₇ Cl	<i>o</i> -Chlorotoluene.....	1.56 C	273 DR 1.56	
C ₇ H ₇ Cl	<i>p</i> -Chlorotoluene.....	2.21 B	273 DR 2.21	

^a Mixture of *ee* and *aa* conformational isomers.

^b Mixture of keto and enol forms.

^c $\mu = 1.11$ D at 328 °K; 1.22 D at 476 °K.

^d Recalculated from the original data.

7.2. Selected dipole moments (compounds containing carbon)—Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C ₇ H ₇ F	<i>o</i> -Fluorotoluene.....	1.37 C	194 DR 1.37	
C ₇ H ₇ F	<i>m</i> -Fluorotoluene.....	1.86 C	194 DR 1.86	
C ₇ H ₇ F	<i>p</i> -Fluorotoluene.....	2.00 C	194 DR 2.00	
C ₇ H ₇ NO ₃	<i>o</i> -Nitro(methoxy)benzene.....	4.83 Bi	120 DR 4.83	
C ₇ H ₇ NO ₃	<i>m</i> -Nitro(methoxy)benzene.....	4.55 Bi	120 DR 4.55	
C ₇ H ₇ NO ₃	<i>p</i> -Nitro(methoxy)benzene.....	5.26 B	120 DR 5.26	
C ₇ H ₈	1,3,5-Cycloheptatriene.....	0.25 C	554 MW 0.25	
C ₇ H ₈	Toluene.....	0.36 C	142 DT 0.36 074 DT 0.36	
C ₇ H ₈ O	Phenylmethanol (benzyl alcohol).....	1.71 C	288 DR 1.71	
C ₇ H ₈ O	Methoxybenzene (anisole).....	1.38 C	120 DR 1.38	
C ₇ H ₉ NO	<i>o</i> -Amino(methoxy)benzene.....	1.61 Ci	148 DR 1.61	
C ₇ H ₁₀	1,6-Heptadiyne.....	i	559 DR 0.81 ^{a,b}	
C ₇ H ₁₂	1-Heptyne.....	0.86 i	136 DR 0.87 559 DR 0.85 ^b	
C ₇ H ₁₄	Methylcyclohexane.....	(0) Qi	142 DT ≈ 0	
C ₇ H ₁₄ O	Methoxycyclohexane.....	1.35 Di	120 DR 1.35	
C ₇ H ₁₄ O ₂	Pentyl acetate (<i>n</i> -amyl acetate).....	1.75 Ci	066 DT 1.75	
C ₇ H ₁₅ Br	1-Bromoheptane.....	2.16 Ci	105 DR 2.16	
C ₇ H ₁₆	Heptane.....	≤ 0.1 Di	098 DT ≈ 0 090 DT ≈ 0	112, 020
C ₈ H ₄ N ₂	<i>p</i> -Dicyanobenzene.....	0 S	131 DT 0	
C ₈ H ₈	Styrene.....	(0) Q	164 DR ~ 0	
C ₈ H ₈ O	Acetylbenzene (acetophenone).....	3.02 B	097 DT 3.02	
C ₈ H ₈ O ₂	2,5-Dimethyl-1,4-cyclohexadienedione.....	0 S	131 DT 0	
C ₈ H ₉ NO ₂	Methyl (<i>o</i> -aminophenyl)formate.....	x Q	018
C ₈ H ₉ NO ₂	Methyl (<i>m</i> -aminophenyl)formate.....	x Q	018
C ₈ H ₉ NO ₂	Methyl (<i>p</i> -aminophenyl)formate.....	x Q	018
C ₈ H ₁₀	Ethylbenzene.....	0.59 C	142 DT 0.59	
C ₈ H ₁₀	<i>o</i> -Xylene.....	0.62 C	156 DR 0.62 ^c	
C ₈ H ₁₀	<i>p</i> -Xylene.....	0 S	156 DR 0	
C ₈ H ₁₀ O	Ethoxybenzene (phenetole).....	1.45 Di	120 DR 1.45	
C ₈ H ₁₁ N	(Dimethylamino)benzene.....	1.68 D	120 DR 1.68	
C ₈ H ₁₂	1,7-Octadiyne.....	i	559 DR 0.88 ^{a,b}	
C ₈ H ₁₂ O ₂	Tetramethylcyclobutane-1,3-dione.....	0 S	131 DT 0	

^a At 308 °K.

^b An allowance has been made for vibrational polarization. See reference 559.

^c The vibrational polarization plus electronic polarization was set equal to the total polarization for *p*-xylene.

7.2. Selected dipole moments (compounds containing carbon)—Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C ₈ H ₁₂ O ₂	Ethyl 2,4-hexadienoate (ethyl sorbate).	(2.07) Qi	166 DR 2.07	
C ₈ H ₁₄ O ₄	Diethyl butanedioate (diethyl succinate).	i	064 DR (a)	
C ₈ H ₁₆	Ethylcyclohexane.....	(0) Q	142 DT ≈ 0	
C ₈ H ₁₈	Octane.....	≤ 0.1 Di	157 DR ≈ 0	
C ₈ H ₁₈ O	Dibutyl ether.....	1.17 Ci	119 DT 1.17	
C ₉ H ₇ N	Quinoline.....	2.29 C	329 DR 2.29	
C ₉ H ₇ N	Isoquinoline.....	2.73 C	329 DR 2.73	
C ₉ H ₁₀ O ₂	Ethyl phenylformate (ethyl benzoate)..	2.00 Ci	097 DR 2.00	
C ₉ H ₁₂	Isopropylbenzene.....	(0.79) Q	142 DR 0.79	
C ₉ H ₁₂ O ₈	Tetrakis(methyl carboxylate)methane.	x Q		068
C ₉ H ₁₄	1,8-Nonadiyne.....	i	559 DR 1.09 ^{b,c}	
C ₉ H ₁₈	Isopropylcyclohexane.....	(0) Q	142 DT ≈ 0	
C ₁₀ H ₈	Azulene.....	0.80 B	575 MW 0.796	
C ₁₀ H ₁₄	<i>t</i> -Butylbenzene.....	(0.83) Q	142 DR 0.83	
C ₁₀ H ₁₄ BeO ₄	Bis(2,4-pentanedionato) beryllium.....	0 S	131 DT 0	
C ₁₀ H ₁₈ O	1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane.	1.42 D	255 DR 1.42	
C ₁₀ H ₂₀	<i>t</i> -Butylcyclohexane.....	(0) Q	142 DT ≈ 0	
C ₁₁ H ₁₆	<i>p</i> - <i>t</i> -Butyltoluene.....	x Q		142
C ₁₂ H ₈ Br ₂ O	Bis(<i>p</i> -bromophenyl) ether.....	1.02 D	132 DR 1.02	
C ₁₂ H ₉ BrO	<i>p</i> -Bromophenoxybenzene.....	1.98 C	132 DR 1.98	
C ₁₂ H ₉ NO ₃	<i>p</i> -Nitrophenoxybenzene.....	4.54 B	132 DR 4.54	
C ₁₂ H ₁₀	Acenaphthene.....	(0.85) Q	347 DR 0.93 310 DR 0.81	
C ₁₂ H ₁₀	Phenylbenzene (diphenyl).....	0 S		029, 030
C ₁₂ H ₁₀ O	Diphenyl ether.....	(1.3) Q	120 DR 1.43 132 DR 1.23	018
C ₁₃ H ₁₀ O	Diphenyl carbonyl.....	x Q		018
C ₁₃ H ₁₁ BrO	<i>p</i> -Bromophenoxy- <i>p</i> -toluene.....	2.45 C	132 DR 2.45	
C ₁₃ H ₁₂	Diphenylmethane.....	x Q		018
C ₁₃ H ₂₀ O ₈	Tetrakis(acetoxymethyl)methane.....	x Q		068
C ₁₄ H ₁₄ O	Bis(<i>p</i> -tolyl) ether.....	1.54 C	132 DR 1.54	
C ₁₅ H ₂₁ AlO ₆	Tris(2,4-pentanedionato) aluminum....	0 S	131 DT 0	
C ₁₅ H ₂₁ CrO ₆	Tris(2,4-pentanedionato) chromium (III).	0 S	131 DT 0	
C ₁₅ H ₂₁ FeO ₆	Tris(2,4-pentanedionato) iron (III).....	0 S		131
C ₂₀ H ₂₈ O ₈ Th	Tetrakis(2,4-pentanedionato) thorium.	0 S		131

^a $\mu = 2.35$ D at 430 °K; 2.41 D at 519 °K.

^b At 308 °K.

^c An allowance for vibrational polarization has been made. See reference 559.

7.3. Appendix I. Variation of Dipole Moment With Vibrational State

The following table summarizes the best available information on the vibrational dependence of dipole moments. Only those cases are included where the precision of the measurement was high enough to make a meaningful comparison of the dipole moment in different vibrational states. A few other cases have been reported in the literature, but the changes were not felt to be experimentally significant. All results in this table were obtained from Stark effect measurements.

The table includes the original investigator's estimate of the precision of his measurements. Since very few authors have specified the statistical estimator used in stating their precision, the precision entries for different compounds are in general not comparable. However, the data in

this table on different vibrational states of a single compound were always obtained by the same investigator on the same apparatus. The precision quoted by the investigator can thus be regarded as a rough indication of the reproducibility of a measurement on a given vibrational state. Since systematic errors should be virtually the same for all states, the quoted precision gives an idea of the significance of the variation of the dipole moment with vibrational state.

It should be emphasized that the accuracy of the dipole moments given in this table is much lower than the precision. In most cases the uncertainty resulting from possible systematic errors is at least an order of magnitude greater than the precision which is quoted.

APPENDIX I. *Variation of dipole moment with vibrational state*

Compound	Vibrational state	Dipole moment (debyes)	Precision (debyes)	References
BaO – Barium oxide.....	$v=0$	7.954	0.002	526, 500
	$v=1$	7.997	0.002	
	$v=2$	8.039	0.002	
	$v=3$	8.079	0.002	
BrK – Potassium bromide.....	$v=0$	10.41	0.02	274
	$v=2$	9.93	0.02	
⁷⁹ Br ⁶ Li – Lithium bromide.....	$v=0$	7.2680	0.0001	535
	$v=1$	7.3523	0.0001	
	$v=2$	7.4377	0.0001	
⁸¹ Br ⁶ Li – Lithium bromide.....	$v=0$	7.2678	0.0001	535
	$v=1$	7.3521	0.0001	
	$v=2$	7.4376	0.0001	
ClCs – Cesium chloride.....	$v=0$	10.420 ^a	0.001	341
	$v=1$	10.476	0.001	
ClK – Potassium chloride.....	$v=0$	10.2688 ^b	0.001	591
	$v=1$	10.3288	0.001	
	$v=2$	10.3877	0.001	

^a Calculated from the equation $\mu_v = 10.42 + 0.056 v$, which was obtained from measurements on the $v=0$ through $v=6$ states.

^b Different values are reported in reference 282 but are believed to be of lower accuracy and precision.

APPENDIX I. Variation of dipole moment with vibrational state—Continued

Compound	Vibrational state	Dipole moment (debyes)	Precision (debyes)	References
³⁵ Cl ⁶ Li—Lithium chloride.....	<i>v</i> =0	7.1195 ^a	0.0006	537
	<i>v</i> =1	7.2069	0.0008	
	<i>v</i> =2	7.2964	0.0012	
	<i>v</i> =3	7.3865	0.0018	
³⁷ Cl ⁶ Li—Lithium chloride.....	<i>v</i> =0	7.1192 ^a	0.0008	537
	<i>v</i> =1	7.2071	0.0012	
	<i>v</i> =2	7.2972	0.0014	
ClNa—Sodium chloride.....	<i>v</i> =0	9.002	0.004	473a
	<i>v</i> =1	9.060	0.004	
	<i>v</i> =2	9.119	0.004	
CsF—Cesium fluoride.....	<i>v</i> =0	7.8750 ^b	0.0002	341
	<i>v</i> =1	7.9472	0.0002	
¹⁹ F ⁶ Li—Lithium fluoride.....	<i>v</i> =0	6.3276 ^c	0.0001	527
	<i>v</i> =1	6.4151	0.0001	
	<i>v</i> =2	6.5034	0.0001	
	<i>v</i> =3	6.5933	0.0001	
FNa—Sodium fluoride.....	<i>v</i> =0	8.1558	0.0001	536
	<i>v</i> =1	8.2209	0.0001	
	<i>v</i> =2	8.2867	0.0001	
FRb—Rubidium fluoride.....	<i>v</i> =0	8.5465	0.0002	591
	<i>v</i> =1	8.6135	0.0002	
	<i>v</i> =2	8.6810	0.0002	
FTl—Thallium fluoride.....	<i>v</i> =0	4.2282	0.0001	397
	<i>v</i> =1	4.2971	0.0001	
	<i>v</i> =2	4.3665	0.0004	
HLi—Lithium hydride.....	<i>v</i> =0	5.882	0.003	442
	<i>v</i> =1	5.990	0.003	
¹²⁷ I ⁶ Li—Lithium iodide.....	<i>v</i> =0	7.4285	0.0002	552
	<i>v</i> =1	7.5120	0.0002	
OSr—Strontium oxide.....	<i>v</i> =0	8.900	0.003	562
	<i>v</i> =1	8.874	0.003	

^a Slightly different values have been reported in reference 591, but the change with vibrational state is not significantly different.

^b Calculated from the equation $\mu_v = 7.875 + 0.0722 v$, which was obtained from measurements on the *v*=0 through *v*=4 states.

^c Essentially the same values have been reported in reference 591.

APPENDIX I. *Variation of dipole moment with vibrational state*—Continued

Compound	Vibrational state	Dipole moment (debyes)	Precision (debyes)	References
O ₂ S—Sulfur dioxide.....	000	1.615	(a)	487b
	010	1.575		
Carbon compounds:				
COSe—Carbonyl selenide.....	000	0.754	(b)	199
	100	0.728		
	010	0.730		
C ₂ H ₂ O—Methylene carbonyl (ketene).....	$v=0^c$	1.414	0.010	261
	$v_7=1$	1.430	0.012	
	$v_8=1$	1.386	0.010	
	$v_9=1$	1.387	0.010	

^a Precision was not stated.

^b Precision was not stated but is estimated to be about 1 percent. Because of a probable systematic error in calibration, all values are about 3 percent high.

^c The vibrational assignment has been revised in accordance with A. P. Cox and A. S. Esbitt, *J. Chem. Phys.* **38**, 1636 (1963).

7.4. Appendix II. Isotopic Dependence of Dipole Moment

This table lists molecules in which isotope shifts in the dipole moment have been accurately measured by microwave or molecular beam techniques. All measurements refer to the ground vibrational state. As in appendix I, only those measurements are included which are felt to be precise enough to give an experimentally significant difference in dipole moments of different isotopic species. This requires that the precision of the measurement be

better than 0.01 D. Other cases of measurements on several isotopic species have been reported in the literature, but the uncertainties were too large to give meaningful shifts. Dielectric measurements of deuterium isotope shifts have been reported in HCl (128) and NH₃ (096).

The comments on precision and accuracy made in appendix I apply to this table.

APPENDIX II. *Isotopic dependence of dipole moment*

Compound	Isotopic species	Dipole moment (debyes)	Precision (debyes)	Reference
Lithium bromide.....	⁷⁹ Br ⁶ Li.....	7.2680 ^a	0.0001	535
	⁸¹ Br ⁶ Li.....	7.2678	0.0001	
	⁷⁹ Br ⁶ Li.....	7.2680	0.0002	591
	⁷⁹ Br ⁷ Li.....	7.2648	0.0002	
Lithium chloride.....	³⁵ Cl ⁶ Li.....	7.1195 ^a	0.0006	537
	³⁷ Cl ⁶ Li.....	7.1192	0.0008	
Lithium fluoride.....	¹⁹ F ⁶ Li.....	6.3275	0.0002	591
	¹⁹ F ⁷ Li.....	6.3248	0.0002	
Thallium fluoride.....	¹⁹ F ²⁰⁵ Tl.....	4.2282 ^b	0.000001	397
	¹⁰ F ²⁰³ Tl.....	4.2282	0.000001	
Lithium hydride.....	¹ H ⁶ Li.....	5.884	0.003	442
	¹ H ⁷ Li.....	5.882	0.003	
Carbon compounds:				
Trifluoromethane.....	¹² C ¹ H ¹⁰ F ₃	1.6460	0.001	587
	¹² C ² H ¹⁹ F ₃	1.6470 ^c	0.001	
Fluoromethane.....	¹² C ¹ H ₃ ¹⁹ F.....	1.8471	0.001	587
	¹² C ² H ₃ ¹⁹ F.....	1.8583	0.001	
Methyl germane.....	¹² C ¹ H ₃ ⁷⁰ Ge ¹ H ₃	0.6425	0.001	587
	¹² C ¹ H ₃ ⁷⁴ Ge ¹ H ₃	0.6420	0.001	
	¹² C ¹ H ₃ ⁷⁰ Ge ² H ₃	0.6295	0.001	
	¹² C ¹ H ₃ ⁷⁴ Ge ² H ₃	0.6298	0.001	
	¹² C ² H ₃ ⁷⁰ Ge ¹ H ₃	0.6548	0.001	
	¹² C ² H ₃ ⁷⁴ Ge ¹ H ₃	0.6539	0.001	
Methyl silane.....	¹² C ¹ H ₃ ²⁸ Si ¹ H ₃	0.7351	0.001	587
	¹² C ¹ H ₃ ²⁸ Si ² H ₃	0.7236	0.001	
1,1-Difluoroethylene.....	¹ H ₂ ¹² C ¹² C ¹⁹ F ₂	1.385	0.001	587
	² H ₂ ¹² C ¹² C ¹⁹ F ₂	1.391	0.001	

APPENDIX II. *Isotopic dependence of dipole moment—Continued*

Compound	Isotopic species	Dipole moment (debyes)	Precision (debyes)	Reference
Propyne.....	$^{12}\text{C}^1\text{H}_3\text{C}^{12}\text{C}^1\text{H}$	0.781	0.001	587
	$^{12}\text{C}^1\text{H}_3\text{C}^{12}\text{C}^2\text{H}$	0.768	0.001	
	$^{12}\text{C}^2\text{H}_3\text{C}^{12}\text{C}^1\text{H}$	0.784	0.001	
	$^{12}\text{C}^2\text{H}_3\text{C}^{12}\text{C}^2\text{H}$	0.772	0.001	
Propane.....	$^{12}\text{C}^1\text{H}_3\text{C}^{12}\text{C}^1\text{H}_2\text{C}^1\text{H}_3$	0.0848	0.001	
	$^{12}\text{C}^1\text{H}_3\text{C}^{12}\text{C}^2\text{H}_2\text{C}^1\text{H}_3$	0.0948	0.001	
	$^{12}\text{C}^2\text{H}_3\text{C}^{12}\text{C}^1\text{H}_2\text{C}^2\text{H}_3$	0.0758	0.001	
2-Methylpropane.....	$(^{12}\text{C}^1\text{H}_3)_3\text{C}^1\text{H}$	0.1320	0.0006	432
	$(^{12}\text{C}^1\text{H}_3)_3\text{C}^2\text{H}$	0.1406	0.0006	

^a See also appendix I.

^b $\mu(^{19}\text{F}^{203}\text{Tl}) - \mu(^{19}\text{F}^{205}\text{Tl}) = (33 \pm 3) \times 10^{-6}$ D.

^c The direction of the isotope shift is felt to be significant.

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