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ALEXANDER B. TROWBRIDGE, *Secretary*,
U. S. NATIONAL BUREAU OF STANDARDS · A. V. ASTIN, *Director*

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, looseleaf 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:

Category	*Title*
1	General
2	Nuclear Properties
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5	Thermodynamic and Transport Properties
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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.*

Contents

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

Ralph D. Nelson, Jr., David R. Lide, Jr., and Arthur A. Maryott

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 tablulated, 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, ($1\ D=10^{-18}$ electrostatic units of charge × centimeters). The conversion factor to the Système International is $1\ D=3.33564\times10^{-24}$ coulomb-meter.

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 reanalyzed. 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	±1% or, for $\mu < 1.0$ D, ±0.01 D
B	±2% or, for $\mu < 1.0$ D, ±0.02 D
C	±5% or, for $\mu < 1.0$ D, ±0.05 D
D	±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

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

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 temperature. 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 $M=J, J-1, \ldots, -J$. 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

$$\Delta W=(A+BM^2)E^2. \tag{2}$$

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 $\boldsymbol{\mu}$ 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

$$\Delta W=\pm CME. \tag{3}$$

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 complicated, 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 CH_3CN (3.918 D), CH_3F (1.847 D), and CHF_3 (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 microwave 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

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

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 (°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 $n \geqslant 3$).

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

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

if B is given in cm^3 mol^{-1} °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

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

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

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

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.

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[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_2O_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_2H_6	Diborane	0 S	102 DT 0	
$B_3H_6N_3$	Triborotriazine (Borazine)	0 S	102 DT 0.7[b]	
B_5H_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_3Si	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_2Hg	Mercury dibromide	0 S	095 DT 0	
Br_4Sn	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 $^{1}H_2\,^{2}H^{75}As$.

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

[c] For $^{2}H^{79}Br$.

[d] For $^{79}Br^{6}Li$.

[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_3Si	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_2F_3P	Dichlorotrifluorophosphorus	0.68 C	561 DT 0.68	
Cl_2H_2Si	Dichlorosilane	1.17 B	129 DT 1.17	
Cl_2Hg	Mercury dichloride	0 S	095 DT 0	

[a] Calculated from microwave intensities.

[b] For $^{37}Cl^{74}Ge^{1}H_3$.

[c] For $^{35}Cl^{6}Li$.

[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_2OS	Thionyl chloride	1.45	B	143	DT	1.45	
Cl_2O_2S	Sulfuryl chloride	1.81	B	143	DT	1.81	
Cl_3F_2P	Trichlorodifluorophosphorus	0	S	561	DT	0	
Cl_3HSi	Trichlorosilane	0.86	B	129	DT	0.86	
Cl_3P	Phosphorus trichloride	0.78	C	072	DT	0.78	
Cl_4FP	Tetrachlorofluorophosphorus	0.21	B	567	NR	0.21	
Cl_4Ge	Germanium tetrachloride	0	S	131	DT	0	
Cl_4Si	Silicon tetrachloride	0	S	298	DT	0	
Cl_4Sn	Tin tetrachloride	0	S	131	DT	0	
Cl_4Ti	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	465, 462
				163	DT	1.91	
				176	DT	1.91	
				532	MB	1.83	
FH_3Si	Fluorosilane	1.27	B	218	MW	1.268	
FH_5Si_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]	309, Vib, Iso, 268
				591	MB	6.325	
$FMnO_3$	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	501, Vib
				528	MB	8.19	
FO_3Re	Perrhenyl fluoride	0.85	D	406	MW	0.85[b]	385
FRb	Rubidium fluoride	8.55	A	382	MB	8.80	Vib
				591	MB	8.5465	
FTl	Thallium fluoride	4.23	A	397	MB	4.2282	374, 380, Vib, Iso
				379	MW	3.99	
F_2HN	Difluoramine	1.92	A	513	MW	1.921 ↗	
F_2H_2Si	Difluorosilane	1.55	A	353	MW	1.55	
F_2N_2	*cis*-Difluorodiazine	0.16	A	510	MW	0.16	
F_2O	Oxygen difluoride	0.297	A	460	MW	0.297	417
				419	DR	0.4	

[a] For $^{19}F^6Li$.

[b] In excited vibrational state $v_5=1$.

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

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
F_2OS	Thionyl fluoride	1.63 A	290 MW 1.627 ↗	
F_2O_2	Dioxygen difluoride	1.44 C	478 MW 1.44	
F_2O_2S	Sulfuryl fluoride	1.12 B	355 MW 1.116	256
F_2S_2	Sulfur monofluoride ($S=SF_2$ isomer)	1.03 C	536a MW 1.03 ↗	
F_2S_2	Sulfur monofluoride (FSSF isomer)	1.45 B	536a MW 1.45	
F_2Si	Silicon difluoride	1.23 B	571 MW 1.23	
F_3HSi	Trifluorosilane	1.27 B	275 MW 1.27	257
F_3N	Nitrogen trifluoride	0.235 A	297 MW 0.236 275 MW 0.235 [a] 115 DT 0.25 102 DT 0.22	
F_3NS	Nitridotrifluorosulfur	1.91 B	481 MW 1.91	
F_3OP	Phosphoryl fluoride	1.76 B	275 MW 1.78 258 MW 1.70 216 MW 1.735	
F_3P	Phosphorus trifluoride	1.03 A	275 MW 1.03 219 MW 1.030	
F_3PS	Thiophosphoryl fluoride	0.64 B	258 MW 0.636	
F_4N_2	Tetrafluorohydrazine, *gauche* conformation.	0.26 B	405 MW 0.26	
F_4S	Sulfur tetrafluoride	0.632 A	498 MW 0.632 419 DR 1.0	
F_4Si	Silicon tetrafluoride	0 S	094 DT 0	
F_5P	Phosphorus pentafluoride	0 S	123 DT 0	
F_5I	Iodine pentafluoride	2.18 C	326 DR 2.18	
F_6S	Sulfur hexafluoride	0 S	546 DT 0 446 DT 0 094 DT 0	149, 133
F_6Se	Selenium hexafluoride	0 S	....	149
F_6Te	Tellurium hexafluoride	0 S	....	149
F_6U	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 $^{19}F_3{}^{15}N$.

[b] For $^{2}H^{127}I$.

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	322, 568a
			455 MW 1.65	
			506 MW 1.60	
$H_2N_2O_2$	Nitroamine (nitramide)	(3.6) Q	522 MW 3.57[b]	
H_2O	Water	1.85 A	062 DT 1.85	001, 023, 033a, 044, 091, 092, 173, 174, 178, 179, 197, 209, 252, 539
			097 DT 1.84	
			106 DT 1.84	
			157 DT 1.85	
			253 DT 1.85	
			594 MW 1.85	
H_2O_2	Hydrogen peroxide	2.2 D	323 MW 2.26	301
H_2S	Hydrogen sulfide	0.97 A	561aMW 0.974	234, 015
			344 DT 0.98	
			027 DT 0.92	
			250 DT 0.89	
H_2Se	Hydrogen selenide	x Q	331 MW 0.24	369, 390, 414
			368 MW 0.62	
H_3N	Ammonia	1.47 A	230 MW 1.468	168, 161, 561, 001, 016, 040, 078, 493, 047 055
			013 DT 1.47	
			096 DT 1.47	
			170 DT 1.46	
			182 DT 1.44	
			342 DT 1.44	
H_3P	Phosphine	0.58 A	285 MW 0.575[c]	
			375 MW 0.576	
			239 MW 0.55	
			016 DT 0.55	
H_3Sb	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 $^2H^2H_2P$ and $^1H_2{}^2HP$.

[d] For $^1H_2{}^2H^{121}Sb$.

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

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
H_4N_2	Hydrazine	1.75 C	479 MW 1.75	
H_4Si	Silane	0 S	094 DT 0	
H_6OSi_2	Disilyl ether (disiloxane)	0.24 B	548 DT 0.24	
H_6Si_2	Disilane	0 S	094 DT 0	
H_9NSi_3	Trisilylamine	$\leqslant$0.1 D	524 DT $\approx$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_4Sn	Tin tetraiodide	0 S	....	131
NO	Nitrogen monoxide (nitric oxide)	0.153 A	376 MW 0.158	075
			407 NR 0.148	
			094 DT 0.16	
NO_2	Nitrogen dioxide	0.316 A	508 MW 0.316	116
			533 MW 0.294[b]	
			139 DT 0.29	
			081 DT 0.39	
N_2O	Dinitrogen oxide (nitrous oxide)	0.167 A	219 MW 0.167	202, 045, 031, 015
			187 MW 0.16	
			094 DT 0.17	
			083 DT 0.14	
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_2S	Sulfur dioxide	1.63 A	231 MW 1.60	566, 015, 010, 001, 003, 240, Vib
			487bMW 1.615	
			126 DT 1.59	
			213 DT 1.63	
			344 DT 1.63	
			013 DT 1.63	
O_3	Ozone	0.53 B	286 MW 0.53	279, 260, 236, 330
			209 DT 0.52	
O_3S	Sulfur trioxide	0 S	126 DT 0	
O_4Os	Osmium tetroxide	0 S	149 DT 0	

[a] For $^{127}I^{6}Li$.

[b] For $^{15}N^{16}O_2$.

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_2F_2	Dibromodifluoromethane	0.66 C	314 DT 0.66	133
$CClF_3$	Chlorotrifluoromethane	0.50 A	434 NR 0.496	475, 450, 209, 133
			451 MW 0.50	
			343 NR 0.50	
			314 DT 0.46	
$CClN$	Cyanogen chloride	2.82 B	219 MW 2.82[a]	180
CCl_2F_2	Dichlorodifluoromethane	0.51 C	076 DT 0.51	209, 133
CCl_2O	Carbonyl chloride (phosgene)	1.17 A	477 MW 1.17	
			472 DT 1.18	
			088 DT 1.19	
CCl_2S	Thiocarbonyl chloride	0.29 C	143 DT 0.29	
CCl_3F	Trichlorofluoromethane	0.45 C	076 DT 0.45	133
CCl_3NO_2	Trichloronitromethane	1.89 C	088 DR 1.89	
CCl_4	Carbon tetrachloride	0 S	298 DT 0	112, 012, 115
			113 DT 0	
CFN	Cyanogen fluoride	2.17 C	523 MW 2.17	439
CF_2	Carbon difluoride	0.46 B	588 MW 0.46	
CF_2O	Carbonyl fluoride	0.95 A	483 MW 0.95	
CF_3I	Iodotrifluoromethane	0.92 C	314 DT 0.92	
			305 MW 1.0	
CF_3NO	Triflurornitrosomethane	(0.3) Q	530 DR 0.31	
CF_3NO_2	Trifluoronitromethane	1.44 C	576 MW 1.44	
CF_4	Carbon tetrafluoride	0 S	115 DT 0	133
			102 DT 0	
			546 DT 0	
CN_4O_8	Tetranitromethane	0 S		131
CO	Carbon monoxide	0.112 A	375 MW 0.112	019, 015, 002, 004, 558,[b] 487a
			344 DT 0.14	
			094 DT 0.10	
			182 DT 0.12	
			027 DT 0.10	
COS	Carbonyl sulfide	0.712 A	360 MB 0.7124	200, 566, 162, 180
			525 MW 0.7120	
			222 MW 0.7085	
			246 MW 0.712	
			175 DT 0.72	
			027 DT 0.67	
$COSe$	Carbonyl selenide	0.73 B	199 MW 0.73	Vib

[a] For $^{12}C^{36}Cl^{14}N$.

[b] $\mu = 1.38 \pm 0.02$ D. in the excited $a^3\Pi$ 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	001, 004, 013, 015, 019, 041, 056, 094, 115
			050 DT 0	
			125 DT 0	
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	487, 133, 441
			076 DT 1.41	
$CHCl_2F$	Dichlorofluoromethane	1.29 B	076 DT 1.29	133
$CHCl_3$	Trichloromethane (chloroform)	1.01 B	153 DT 1.01	446, 112, 024, 012
			113 DT 1.02	
$CHFO$	Formyl fluoride	2.02 A	430 MW 2.02 ↗	420
CHF_3	Trifluoromethane	1.65 A	587 MW 1.646	Iso, 191
			246 MW 1.646	
			446 DT 1.65	
			257 MW 1.65	
			314 DT 1.62	
			102 DT 1.60	
CHN	Hydrogen cyanide	2.98 A	415 MW 2.986	221, 037
			275 MW 3.01	
			088 DT 2.95	
			115 DR 3.00	
			050 DT 2.91	
$CHNO$	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_2Br_2	Dibromomethane	1.43 B	153 DT 1.43	022
			271 DT 1.43	
CH_2ClF	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_2ClNO_2	Chloronitromethane	2.91	B	157	DR	2.91	
CH_2Cl_2	Dichloromethane	1.60	B	266	MW	1.63	112, 022, 012
				153	DT	1.57	
				113	DT	1.54	
CH_2F_2	Difluoromethane	1.97	A	262	MW	1.97	
CH_2N_2	Cyanogen amide (cyanamide)	4.27	C	413	MW	4.3	
				494	MW	4.24 [a]	
CH_2N_2	Diazomethane	1.50	A	493a	MW	1.50	377
CH_2N_2	Diazirine	1.59	C	490	MW	1.59	
CH_2O	Methanal (formaldehyde)	2.33	A	246	MW	2.34	534, 184, 584 [b]
				428	MW	2.33	
				237	MW	2.31	
				160	DR	2.29	
CH_2O_2	Methanoic acid (formic acid)	1.41	A	480	MW	1.415 ↗	378
				058	DR	1.52	
				130	DR	1.4	
CH_3BF_2	Methyl difluoroborane	1.66	B	364	MW	1.67	
				342	DT	1.62	
CH_3BO	Carbonyl borane	1.80	B	198	MW	1.795 [c]	
CH_3Br	Bromomethane	1.81	A	219	MW	1.81	100, 042, 566
				089	DT	1.80	
				113	DR	1.81	
				271	DT	1.83	
				118	DT	1.76	
CH_3Cl	Chloromethane	1.87	A	193	MW	1.87	100, 042, 043, 024, 012, 035
				219	MW	1.88	
				113	DR	1.89	
				038	DT	1.87	
				062	DT	1.87	
CH_3F	Fluoromethane	1.85	A	511	MW	1.8555	Iso, 191, 275
				113	DT	1.85	
				089	DT	1.81	
				587	MW	1.8471	
CH_3F_3Ge	Methyl trifluorogermane	x	Q	424	MW	3.8	

[a] For $^{12}C^{2}H_2{}^{14}N_2$.
[b] $\mu = 1.56 \pm 0.07$ D in the excited $^1A_2$ electronic state.
[c] For $^{12}C^{1}H_3{}^{10}B^{16}O$.

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

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
CH_3I	Iodomethane	1.62 B	321 DT 1.64	100, 042, 021
			113 DR 1.62	
			089 DT 1.60	
			219 MW 1.65	
			118 DR 1.67	
CH_3NO	Hydroxyliminomethane (formaldoxime).	0.44 A	484 MW 0.44 ↗	
			491 MW 0.46 ↗	
CH_3NO	Formyl amide (formamide)	3.73 B	351 MW 3.73 ↗	
			064 DR 3.25	
CH_3NOS	Methyl sulfinylamine	1.70 B	572 MW 1.70	
CH_3NO_2	Nitritomethane (methyl nitrite)	i	507 DR (a)	
CH_3NO_2	Nitromethane	3.46 A	340 MW 3.48	
			298 DT 3.43	
			088 DT 3.44	
			118 DR 3.57	
CH_3NO_3	Methyl nitrate	3.12 B	448 MW 3.12	
CH_3N_3	Methyl azide	2.17 B	589 MW 2.17	
CH_4	Methane	0 S	094 DT 0	012, 078
CH_4F_2Si	Methyl difluorosilane	2.11 A	389 MW 2.11 ↗	
CH_4O	Methanol	1.70 A	140 DT 1.71	141, 229, 280, 001, 172
			113 DT 1.70	
			098 DT 1.70	
			033 DT 1.70	
CH_4S	Methanethiol (methyl mercaptan)	1.52 C	427 MW 1.52 ↗	350, 245
CH_5FSi	Methyl monofluorosilane	1.71 A	387 MW 1.71 ↗	
CH_5N	Methyl amine	1.31 B	354 MW 1.33[b] ↗	263, 137, 052, 055, 047
			170 DT 1.30	
			113 DT 1.26	
			119 DT 1.35	
			062 DT 1.24	
CH_5P	Methyl phosphine	1.10 A	452 MW 1.10	
CH_6Ge	Methyl germane	0.643 A	401 MW 0.635	372, 373, Iso
			444 MW 0.644	
			587 MW 0.6425	
CH_6OSi	Methoxysilane	1.17 B	548 DT 1.17	
CH_6Si	Methyl silane	0.735 A	349 MW 0.73	Iso
			214 MW 0.73	
			587 MW 0.7351	

[a] $\mu = 2.22$ D at 308 °K.

[b] For $^{12}C^{2}H_3{}^{14}N^{2}N_2$.

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

Formula	Compound name	Selected moment (debyes)		Basic references			Other data
CH_6Sn	Methyl stannane	0.68	C	238	MW	0.68	
C_2ClF_3	Chlorotrifluoroethylene	0.40	D	325	DT	0.38	
				344	DR	0.58	
				314	DT	0.40	
C_2ClF_5	Chloropentafluoroethane	0.52	C	314	DT	0.52	133
$C_2Cl_2F_4$	1,2-Dichlorotetrafluoroethane	(0.5)	Qi	336	DT	0.53	133, 416
				344	DT	0.46	
C_2F_3N	Trifluorocyanomethane	1.33	D	499	DR	1.33	
C_2F_6	Hexafluoroethane	0	S				133
C_2F_6O	Bis(trifluoromethyl) ether	0.54	D	314	DT	0.54	
C_2N_2	Dicyanogen (cyanogen)	0	S	115	DT	0	050
C_2N_2S	Dicyano sulfide	3.02	A	569	MW	3.04	
				527a	MW	3.01	
C_2HBr	Bromoacetylene	$\leq$0.10	D	129	DT	0.0[a]	
C_2HCl	Chloroacetylene	0.44	A	204	MW	0.44	
				129	DT	0.45	
C_2HCl_5	Pentachloroethane	0.92	C	201	DT	0.92	
C_2HF	Fluoroacetylene	0.73	C	523	MW	0.73	413, 440
C_2HF_3	Trifluoroethylene	1.40	C	518	MW	1.40	
$C_2HF_3O_2$	Trifluoroethanoic acid (trifluoroacetic acid).	2.28	D	233	DR	2.28	
C_2HF_5	Pentafluoroethane	1.54	C	314	DT	1.54	
C_2H_2	Acetylene	0	S	009	DT	0	540[b]
				094	DT	0	
$C_2H_2Cl_2$	1,1-Dichloroethylene	1.34	A	477	MW	1.34	
$C_2H_2Cl_2$	*cis*-1,2-Dichloroethylene	1.90	B	153	DT	1.90	
$C_2H_2Cl_2F_2$	1,1-Dichloro-2,2-difluoroethane		i	315	DR	(c)	
$C_2H_2Cl_2O$	Chloroacetyl chloride	2.23	Ci	065	DT	2.23	
$C_2H_2Cl_3F$	1,1,2-Trichloro-2-fluoroethane		i	315	DR	(d)	
$C_2H_2Cl_4$	1,1,2,2-Tetrachloroethane	1.32	Ci	201	DT	1.32	
				104	DR	1.36	
C_2H_2FN	Fluorocyanomethane	3.43	C	474	MW	3.43 ↗	
$C_2H_2F_2$	1,1-Difluoroethylene	1.38	A	196	MW	1.366	Iso
				587	MW	1.385	
				445	DR	1.41	
$C_2H_2F_2$	*cis*-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 $^{12}C_2\,^1H^2H$ 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
$C_2H_2N_2O$	1,2,5-Oxadiazole	3.38 A	573 MW 3.38	
$C_2H_2N_2O$	1,3,4-Oxadiazole	3.04 B	582 MW 3.04	
$C_2H_2N_2S$	1,2,5-Thiadiazole	1.56 A	505 MW 1.565	
$C_2H_2N_2S$	1,3,4-Thiadiazole	3.29 B	468 MW 3.29	
C_2H_2O	Methylene carbonyl (ketene)	1.42 B	261 MW 1.414	Vib
			166 DR 1.45	
			227aDR 1.46	
C_2H_3Br	Bromoethylene	1.42 B	135 DT 1.42	
C_2H_3Cl	Chloroethylene	1.45 B	135 DT 1.45	
			426 MW 1.420[a]	
$C_2H_3ClF_2$	1-Chloro-1,1-difluoroethane	2.14 B	315 DT 2.14	133
C_2H_3ClO	Acetyl chloride	2.72 C	065 DT 2.72	
$C_2H_3ClO_2$	Methyl chloroformate	i	138 DR (b)	
$C_2H_3Cl_3$	1,1,1-Trichloroethane	1.78 B	153 DT 1.79	
			155 DR 1.77	
$C_2H_3Cl_3$	1,1,2-Trichloroethane	i	315 DR (c)	195, 201
C_2H_3F	Fluoroethylene	1.43 A	456 MW 1.427↗	
C_2H_3FO	Acetyl fluoride	2.96 A	409 MW 2.96↗	
$C_2H_3F_3$	1,1,1-Trifluoroethane	2.32 B	219 MW 2.33	
			257 MW 2.28	
			133 DR 2.35	
$C_2H_3F_3$	1,1,2-Trifluoroethane	1.58 B	516 MW 1.58[d]	541,[e] 515,[e] 517,[e] 488
C_2H_3I	Iodoethylene	1.30 D	135 DR 1.30	
C_2H_3N	Cyanomethane (acetonitrile)	3.92 A	275 MW 3.94	208
			446 DR 3.90	
			118 DT 3.96	
			113 DR 3.84	
			592 MW 3.918	
C_2H_3N	Isocyanomethane	3.85 B	275 MW 3.85	
C_2H_3NO	Methyl isocyanate	(2.8) Q	504aMW 2.81[f]	
C_2H_3NS	Methyl thiocyanate	(4.0) Q	568 MW 4.03[f]	
C_2H_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 C_1.
[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_2H_4BrCl	1-Bromo-2-chloroethane	i	063 DR ([a])	
$C_2H_4Br_2$	1,2-Dibromoethane	i	063 DR ([b])	059
			151 DR ([b])	
C_2H_4ClF	1-Chloro-2-fluoroethane, *gauche* conformation.	2.72 C	567aMW 2.72	
C_2H_4ClF	1-Chloro-2-fluoroethane	i	315 DR ([c])	
$C_2H_4ClNO_2$	1-Chloro-1-nitroethane	3.27 B	157 DT 3.27	
$C_2H_4Cl_2$	1,1-Dichloroethane	2.06 B	153 DT 2.06	032
$C_2H_4Cl_2$	1,2-Dichloroethane	i	057 DR ([d])	032, 053, 059, 061
			158 DR ([d])	
			151 DR ([d])	
$C_2H_4Cl_2O$	Bis(chloromethyl) ether	i	312 DR ([e])	
$C_2H_4F_2$	1,1-Difluoroethane	2.27 B	429 MW 2.30↗	
			233 DT 2.24	
C_2H_4Ge	Germyl acetylene	0.136 A	581 MW 0.136	
C_2H_4O	Oxirane (ethylene oxide)	1.89 A	232 MW 1.89	
			026 DT 1.90	
			113 DR 1.91	
			346 DT 1.91	
C_2H_4O	Ethanal (acetaldehyde)	2.69 B	348 MW 2.69↗	
			160 DR 2.72	
			065 DR 2.72	
$C_2H_4O_2$	Ethanoic acid (acetic acid)	1.74 C	058 DR 1.74	049
$C_2H_4O_2$	Methyl methanoate (methyl formate).	1.77 B	394 MW 1.77↗	
C_2H_4S	Thiirane (ethylene sulfide)	1.85 A	232 MW 1.85	
C_2H_4Si	Silyl acetylene	0.316 A	514 MW 0.316	
C_2H_5Br	Bromoethane	2.03 A	118 DT 2.02	042, 112, 100, 021
			089 DT 2.03	
C_2H_5BrO	Bromomethoxymethane	2.05 Ci	312 DR 2.05 [f]	

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[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_2H_5Cl	Chloroethane	2.05	A	371	MW	1.745 [a]	035, 308, 024, 042, 043, 100
				038	DT	2.06	
				062	DT	2.03	
				113	DR	2.07	
				175	DR	1.98	
C_2H_5ClO	2-Chloroethanol	1.78	Ci	064	DR	1.78	
C_2H_5ClO	Chloromethoxymethane		i	315	DR	(b)	
				312	DR	(b)	
C_2H_5F	Fluoroethane	1.94	B	320	MW	1.96 ↗	
				089	DT	1.92	
C_2H_5I	Iodoethane	1.91	B	425	MW	1.77 ↗	021, 042, 100, 112
				089	DT	1.92	
				118	DR	1.90	
C_2H_5N	Iminoethane (ethyleneimine)	1.90	A	281	MW	1.90	
C_2H_5N	Methyliminomethane ($CH_3N=CH_2$)	1.53	B	545	MW	1.53	
C_2H_5NO	Acetyl amine (acetamide)	3.76	Bi	539	DR	3.76	
C_2H_5NO	Methylaminomethanal (*N*-methylformamide).	3.83	Bi	539	DR	3.83	
$C_2H_5NO_2$	Nitritoethane (ethyl nitrite)	2.40	Ci	083	DR	2.38	
				313	DR	2.42	
$C_2H_5NO_2$	Nitroethane	3.65	B	157	DR	3.69	
				118	DR	3.61	
C_2H_6	Ethane	0	S	009	DT	0	
				094	DT	0	
C_2H_6AlCl	Dimethylaluminum chloride	x	Q	...			154
C_2H_6BF	Dimethyl fluoroborane	1.32	C	342	DT	1.32	
C_2H_6O	Ethanol	1.69	Bi	033	DR	1.69	509, 014, 411 140
				060	DT	1.70	
				098	DT	1.68	
C_2H_6O	Dimethyl ether	1.30	A	503	MW	1.302	034, 043
				026	DT	1.30	
				062	DT	1.30	
				113	DT	1.29	
				119	DT	1.31	
				561	DT	1.29	

[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 mements (compounds containing carbon) – Continued

Formula	Compound name	Selected moment (debyes)	Basic references	Other data
C_2H_6OS	Dimethylsulfoxide	3.96 A	532aMW 3.96↗	
$C_2H_6O_2$	1,2-Ethanediol (ethylene glycol)	2.28 Ci	064 DR 2.28	
$C_2H_6O_2S$	Dimethyl sulfoxylate (dimethyl sulfone).	4.49 B	143 DR 4.49	
C_2H_6S	Ethanethiol	1.58 Bi	108 DT 1.58	
C_2H_6S	Dimethyl sulfide	1.50 A	459 MW 1.50	
C_2H_6Si	Silyl ethylene	0.66 A	457 MW 0.662	
$C_2H_7B_5$	2,4-Dicarbaheptaborane	1.32 B	550 MW 1.32	
C_2H_7N	Aminoethane (ethyl amine)	1.22 Ci	206 DT 1.22	052
C_2H_7N	Dimethyl amine	1.03 B	170 DT 1.03	137, 055, 052, 047
			119 DT 1.03	
			062 DT 0.97	
C_2H_7P	Ethyl phosphine	1.17 Bi	352 DT 1.17	
C_2H_7P	Dimethyl phosphine	1.23 A	519 MW 1.23	
$C_2H_8N_2$	1,2-Diaminoethane	1.99 Ci	064 DR 1.99	
C_2H_8Si	Dimethyl silane	0.75 A	458 MW 0.75	
C_2H_8Si	Ethyl silane	0.81 B	436 MW 0.81	
$C_3Cl_3F_3$	1,1,2-Trichloro-3,3,3-trifluoropropene.	1.28 D	273 DR 1.28	
C_3O_2	Dicarbonyl carbon (carbon suboxide).	0 S	352 DT 0	
C_3HF_3	3,3,3-Trifluoropropyne	2.36 B	247 MW 2.36	
C_3HF_7	1,1,2,2,3,3,3-Heptafluoropropane	1.62 Di	325 DT 1.62	
C_3HN	Cyanoacetylene	3.72 A	226 MW 3.6	
			593 MW 3.724	
$C_3H_2N_2$	Dicyanomethane	3.73 A	422 MW 3.735	
C_3H_2O	Propynal	2.47 B	319 MW 2.47↗	585[a]
$C_3H_2O_3$	Vinylene carbonate	4.55 A	304 MW 4.53	
			583 MW 4.57	
C_3H_3Br	3-Bromopropyne	1.54 C	345 DR 1.54	
C_3H_3Cl	3-Chloropropyne	1.68 C	449 MW 1.68↗	381
			345 DR 1.67	
$C_3H_3F_3$	3,3,3-Trifluoropropene	2.45 B	273 DR 2.45	
C_3H_3N	Cyanoethylene	3.87 B	307 MW 3.91↗	
			160 DT 3.83	
C_3H_3NO	Acetyl cyanide	3.45 B	400 MW 3.45↗	
C_3H_3NS	Thiazole	1.62 B	467 MW 1.62	
C_3H_4	Cyclopropene	0.45 A	398 MW 0.454	
C_3H_4	Propyne	0.781 A	136 DR 0.78	257, Iso
			115 DT 0.72	
			275 MW 0.75	
			587 MW 0.781	

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[a] In the excited $^1A''$ 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_3H_4	Propadiene (allene)	0 S	115 DT 0	
$C_3H_4Cl_2$	1,1-Dichlorocyclopropane	1.58 B	473 MW 1.58	
$C_3H_4Cl_2$	1,3-Dichloropropene, bp 104 °C isomer.	i	195 DR 1.79	
$C_3H_4Cl_2$	1,3-Dichloropropene, bp 112 °C isomer.	i	195 DR 1.81	
$C_3H_4Cl_2$	2,3-Dichloropropene	i	195 DR (a)	
$C_3H_4Cl_2O$	1,1-Dichloropropanone	i	311 DR (b)	
$C_3H_4Cl_4$	1,1,2,2-Tetrachloropropane	i	362 DR (c)	302
C_3H_4O	Ethylidene carbonyl (methyl ketene)	1.79 B	590 MW 1.79↗	469
C_3H_4O	Propenal, *trans* conformation (acrolein).	3.12 B	370 MW 3.12↗ 166 DR 3.04[d]	
$C_3H_4O_2$	2-Oxoöxetane (β-propiolactone)	4.18 A	333 MW 4.20↗ 551 MW 4.17	
$C_3H_4O_2$	Vinyl formate	1.49 A	544 MW 1.49↗	
C_3H_5Br	3-Bromopropene	(1.9) Q	020 DR 1.93	
C_3H_5Cl	2-Chloropropene	1.66 B	165 DT 1.66 020 DR 1.66	
C_3H_5Cl	*cis*-1-Chloropropene	1.67 C	529 MW 1.64↗ 165 DR 1.71	
C_3H_5Cl	*trans*-1-Chloropropene	1.97 C	165 DR 1.97	
C_3H_5Cl	3-Chloropropene	1.94 Ci	121 DT 1.90 165 DR 1.98	100, 042
C_3H_5ClO	Chloropropanone	i	065 DR (e)	
$C_3H_5ClO_2$	Ethyl chloroformate	i	138 DR (f)	
$C_3H_5Cl_3$	1,2,2-Trichloropropane	i	362 DR (g)	303
C_3H_5F	*cis*-1-Fluoropropene	1.46 B	470 MW 1.46↗	
C_3H_5F	*trans*-1-Fluoropropene	(1.9) Q	365 MW 1.86[h]	
C_3H_5F	2-Fluoropropene	1.61 B	410 MW 1.61↗	
C_3H_5F	3-Fluoropropene, *cis* conformation	1.76 A	560 MW 1.765↗	
C_3H_5F	3-Fluoropropene, *gauche* 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_3H_5N	Cyanoethane (propionitrile)	4.02 A	402 MW 4.02↗	
			118 DT 4.05	
			160 DR 4.00	
$C_3H_5NO_2$	3-Nitritopropene (allyl nitrite)	i	507 DR (a)	
C_3H_6	Cyclopropane	0 S	113 DT 0	
C_3H_6	Propene	0.366 A	356 MW 0.366↗	
			074 DT 0.35	
			094 DT 0.34	
$C_3H_6Br_2$	1,2-Dibromopropane	i	362 DR (b)	303
$C_3H_6ClNO_2$	1-Chloro-1-nitropropane	3.48 Bi	157 DT 3.48	
$C_3H_6Cl_2$	1,2-Dichloropropane	i	195 DR (c)	
$C_3H_6Cl_2$	1,3-Dichloropropane	2.08 Bi	104 DT 2.08[d]	
$C_3H_6Cl_2$	2,2-Dichloropropane	2.27 C	153 DR 2.27	
C_3H_6O	Oxetane (trimethylene oxide)	1.94 A	418 MW 1.94	317
			346 DT 1.94	
C_3H_6O	Methyl oxirane (propylene oxide)	2.01 A	367 MW 2.01↗	
C_3H_6O	Propanone (acetone)	2.88 A	412 MW 2.90	112
			344 DT 2.88	
			272 DT 2.89	
			026 DT 2.87	
			113 DR 2.87	
			065 DR 2.88	
C_3H_6O	2-Propen-1-ol (allyl alcohol)	1.60 C	099 DT 1.60	
C_3H_6O	Propanal, *cis* conformation (propionaldehyde).	2.52 B	531 MW 2.52↗	
			160 DT 2.72[e]	
$C_3H_6O_2$	Propanoic acid	1.75 Ci	058 DR 1.75	
$C_3H_6O_2$	Methyl acetate	1.72 Ci	138 DT 1.72	
			066 DR 1.72	
$C_3H_6O_2$	Ethyl formate	1.93 Ci	066 DT 1.93	
$C_3H_6O_3$	Dimethyl carbonate	i	122 DR (f)	
$C_3H_6O_3$	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_3H_6S	Thietane (trimethylene sulfide)	1.85 C	577 MW 1.85	
C_3H_6S	Methyl thiirane (propylene sulfide)	1.95 A	504 MW 1.95	
C_3H_7Br	1-Bromopropane	2.18 Ci	118 DR 2.18	100, 042
C_3H_7Br	2-Bromopropane	2.21 C	118 DR 2.21	
C_3H_7Cl	1-Chloropropane	2.05 Bi	062 DT 2.05	112, 100, 043, 042, 053, 035
C_3H_7Cl	2-Chloropropane	2.17 C	118 DR 2.17	
C_3H_7F	1-Fluoropropane, *gauche* conformation.	1.90 C	476 MW 1.90 ↗	
C_3H_7F	1-Fluoropropane, *trans* conformation.	2.05 B	476 MW 2.05 ↗	
C_3H_7I	1-Iodopropane	2.04 Ci	118 DR 2.04	100, 042
C_3H_7N	3-Aminopropene	(1.2) Q	020 DR 1.20	
C_3H_7NO	N,N-Dimethylformamide	3.82 Bi	539 DR 3.82	
C_3H_7NO	Acetyl methylamine (*N*-Methylacetamide).	3.73 Bi	539 DR 3.73	
$C_3H_7NO_2$	1-Nitritopropane (*n*-propyl nitrite)	i	507 DR ([a])	
$C_3H_7NO_2$	2-Nitritopropane (isopropyl nitrite)	i	313 DR ([b])	
$C_3H_7NO_2$	1-Nitropropane	3.66 Bi	118 DR 3.60 155 DR 3.72	
$C_3H_7NO_2$	2-Nitropropane	3.73 B	155 DR 3.73	
C_3H_8	Propane	0.084 A	431 MW 0.083 587 MW 0.085	352, 277, 094, 074, Iso
C_3H_8O	1-Propanol	1.68 Bi	033 DT 1.69 099 DT 1.67	
C_3H_8O	2-Propanol	1.66 Bi	098 DT 1.60 127 DT 1.69	
C_3H_8O	Methoxyethane (methyl ethyl ether)	1.23 Ci	194 DT 1.23	
$C_3H_8O_2$	Dimethoxymethane	i	109 DR ([c])	
C_3H_9Al	Trimethyl aluminum	x Q	....	154
C_3H_9As	Trimethyl arsine	0.86 B	404 MW 0.86	
$C_3H_9BF_3N$	Trimethyl amine—boron trifluoride complex.	(5) Q	438 MW 5	
C_3H_9N	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_3H_9N	1-Aminopropane (*n*-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_3H_9P	Trimethyl phosphine	1.19	A	384	MW	1.192	
$C_3H_{10}Si$	Trimethyl silane	0.525	A	437	MW	0.525	
$C_4Cl_3F_7$	2,2,3-Trichloroheptafluorobutane	(0.9)	Qi	336	DT	0.85	
C_4F_8	Perfluorocyclobutane	0	S	314	DT	0	
C_4F_8O	Perfluoroöxolane (perfluorotetramethylene oxide).	0.56	D	325	DT	0.56	
$C_4F_{10}O$	Perfluoro(ethoxyethane)	0.47	Di	325	DT	0.51	
				314	DT	0.42	
$C_4H_2N_2$	*trans*-1,2-Dicyanoethylene	0	S	......			151
C_4H_4	1-Buten-3-yne	(0.4)	Q	496	MW	0.43[a]	
$C_4H_4Cl_2$	1,4-Dichloro-2-butyne	2.10	Bi	363	DR	2.10	
$C_4H_4F_2$	1,1-Difluoro-1,3-butadiene (*trans* conformation).	1.29	A	549	MW	1.29	
$C_4H_4N_2$	1,2-Dicyanoethane		i	151	DR	(b)	
C_4H_4O	Furan	0.66	A	249	MW	0.664	
				278	DT	0.72	
C_4H_4O	3-Butyne-2-one	(2.4)	Q	521	MW	2.4	
$C_4H_4O_2$	Diketene	3.53	B	160	DR	3.53	
C_4H_4S	Thiophene	0.55	C	278	DT	0.55	
				108	DT	0.56	
C_4H_5Cl	4-Chloro-1,2-butadiene	2.02	Ci	165	DR	2.02	
C_4H_5Cl	1-Chloro-2-butyne	2.19	C	345	DR	2.19	
C_4H_5F	2-Fluoro-1,3-butadiene (*trans* conformation).	1.42	A	486	MW	1.417 ↗	
C_4H_5N	Pyrrole	1.84	C	270	DT	1.84	327
C_4H_5N	*cis*-1-Cyanopropene	4.08	B	502	MW	4.08 ↗	
C_4H_5N	*trans*-1-Cyanopropene	4.50	B	160	DR	4.50	
C_4H_5N	2-Cyanopropene (methacrylonitrile)	3.69	C	166	DR	3.69	
C_4H_6	Cyclobutene	0.132	A	563	MW	0.132	
C_4H_6	1-Butyne	0.80	C	136	DR	0.80	
C_4H_6	1,2-Butadiene	0.403	A	357	MW	0.403 ↗	
C_4H_6	1,3-Butadiene	0	S	159	DT	0[c]	

[a] Component along *a* axis.

[b] μ=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 (debyes)	Basic references	Other data
C_4H_6O	Cyclobutanone	2.99 B	500aMW 2.99	
C_4H_6O	*trans*-2-Butenal (crotonaldehyde)	3.67 Bi	160 DR 3.67	
C_4H_6O	2-Methylpropenal (methacrolein)	2.68 Ci	166 DR 2.68	
C_4H_6O	3-Butene-2-one	3.16 B	557 MW 3.16↗	
$C_4H_6O_2$	2,3 -Butanedione	(0) Qi	151 DT ([a])	063
$C_4H_6O_3$	Acetyl acetate (acetic anhydride)	(2.8) Qi	082 DR 2.8	
C_4H_6S	Divinyl sulfide	1.20 D	165 DR 1.20	
C_4H_7Cl	1-Chloro-2-methylpropene	1.95 Bi	160 DT 1.95 165 DR 1.85	
$C_4H_7Cl_3$	1,1,2-Trichloro-2-methylpropane	1.86 Ci	362 DR 1.86	
C_4H_7F	Fluorocyclobutane	1.94 A	586 MW 1.94	
C_4H_7N	1-Cyanopropane	4.07 Bi	118 DR 4.07	
C_4H_8	1-Butene	0.34 Ci	009 DT 0.38 115 DT 0.30	
C_4H_8	*cis*-2-Butene	0.3 D	344 DT 0.33	
C_4H_8	*trans*-2-Butene	0 S	115 DT 0	
C_4H_8	2-Methylpropene	0.50 A	454 MW 0.503 115 DT 0.49	
$C_4H_8Br_2$	1,2-Dibromo-2-methylpropane	i	362 DR ([b])	
$C_4H_8Cl_2$	1,4-Dichlorobutane	2.22 Ci	195 DR 2.22	
$C_4H_8Cl_2$	1,2-Dichloro-2-methylpropane	i	362 DR ([c])	303
C_4H_8O	Tetrahydrofuran	1.63 C	346 DT 1.63	
C_4H_8O	*cis*-2,3-Dimethyloxirane	2.03 A	464 MW 2.03↗	
C_4H_8O	Butanal	2.72 Bi	160 DR 2.72	
$C_4H_8O_2$	1,4-Dioxane	0 S	111 DT 0 087 DT 0	
$C_4H_8O_2$	Ethyl acetate	1.78 Ci	066 DT 1.78	
C_4H_9Br	1-Bromobutane	2.08 Ci	118 DT 2.08	
C_4H_9Br	2-Bromobutane	2.23 Ci	118 DR 2.23	
C_4H_9Cl	1-Chlorobutane	2.05 Bi	105 DT 2.05 118 DR 2.14	
C_4H_9Cl	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_4H_9Cl	1-Chloro-2-methylpropane	2.00 Ci	155 DT 2.00	
C_4H_9Cl	2-Chloro-2-methylpropane	2.13 B	155 DR 2.13	
C_4H_9F	2-Fluoro-2-methylpropane	1.96 A	384 MW 1.959	269
C_4H_9I	1-Iodobutane	2.12 Ci	118 DR 2.12	
C_4H_9NO	Propanoyl methylamine (N-methylpropionamide).	3.61 Bi	539 DR 3.61	
C_4H_9NO	Acetyl dimethylamine (N,N-dimethylacetamide).	3.81 Bi	539 DR 3.81	
$C_4H_9NO_2$	2-Nitrito-2-methylpropane (t-butyl nitrite).	2.74 Ci	508 DR 2.77 313 DR 2.71	
$C_4H_9NO_2$	1-Nitrobutane	3.59 Bi	118 DR 3.59	
$C_4H_9NO_2$	2-Nitro-2-methylpropane	3.71 B	155 DR 3.71	
C_4H_{10}	Butane	$\leq$ 0.05 Ci	277 DT $\leq$ 0.05	115
C_4H_{10}	2-Methylpropane	0.132 A	384 MW 0.132 337 NR 0.132 277 DT 0.13	432, 115, Iso
$C_4H_{10}O$	1-Butanol	1.66 Bi	099 DT 1.65 033 DT 1.67	112
$C_4H_{10}O$	2-Methylpropan-1-ol (isobutanol)	1.64 C	098 DT 1.64	
$C_4H_{10}O$	Diethyl ether	1.15 Bi	194 DT 1.13 026 DT 1.15 062 DT 1.11 119 DT 1.19	146, 044, 038, 034, 014
$C_4H_{10}S$	Diethyl sulfide	1.54 Ci	108 DT 1.54	
$C_4H_{11}N$	1-Aminobutane (n-butylamine)	(1.0) Qi	228 DT 1.00[a]	
$C_4H_{11}N$	Diethyl amine	0.92 Ci	206 DT 0.92	052
C_5F_{12}	Perfluoropentane	$\leq$ 0.10 Di	233 DT 0[b]	
C_5F_{12}	Perfluoro (2-methylbutane)	$\leq$ 0.10 Di	233 DT 0[b]	
C_5H_5N	Pyridine	2.19 B	329 DT 2.23 289 MW 2.15	
C_5H_5N	1-Cyano-1,3-butadiene	3.90 Ci	166 DR 3.90	
C_5H_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_5H_8	Cyclopentene	0.20 B	555 MW 0.190[a] 492 MW 0.22	
C_5H_8	1-Pentyne	0.81 Ci	136 DR 0.86 559 DR 0.81[b]	
C_5H_8	*trans*-1,3-Pentadiene	0.68 Di	159 DR 0.68	
C_5H_8	2-Methyl-1,3-butadiene (*trans* conformation).	0.25 A	538 MW 0.25 ↗	159
$C_5H_8Br_4$	1,3-Dibromo-2,2-bis(bromomethyl) propane.	x Q	....	068
C_5H_8O	Cyclopentanone	(3.3) Q	399 MW 3.30[c]	
$C_5H_8O_2$	Acetylacetone	Ci	082 DR 3.05[d]	
C_5H_9N	1-Cyanobutane	4.12 Bi	097 DT 4.12	
C_5H_9N	2-Cyano-2-methylpropane	3.95 A	489 MW 3.95	
C_5H_{10}	Ethylcyclopropane	(0.5) Q	020 DR 0.47	
C_5H_{10}	1-Pentene	(0.5) Q	020 DR 0.51	
$C_5H_{10}O_3$	Diethyl carbonate	1.10 Ci	110 DT 1.10	
$C_5H_{11}Br$	1-Bromopentane	2.20 Ci	314 DR 2.20	
$C_5H_{11}Cl$	1-Chloropentane	2.16 Ci	118 DR 2.16	
C_5H_{12}	Pentane	<0.1 Di	277 DT <0.07 352 DT <0.05	098, 020, 112
C_5H_{12}	2-Methylbutane	0.13 C	352 DT 0.13 277 DT 0.1	
C_5H_{12}	2,2-Dimethylpropane	0 S	277 DT 0	
$C_5H_{12}O_2$	Diethoxymethane	i	110 DR ([e])	
$C_5H_{12}O_4$	Tetramethoxymethane	0 Qi	038 DT ≈ 0	030
$C_6H_2Cl_2O_2$	2,5-Dichloro-1,4-cyclohexadienedione	0 S	131 DT 0	
C_6H_4BrF	*p*-Bromofluorobenzene	(0.5) Q	156 DR 0.5	
$C_6H_4ClNO_2$	*o*-Chloronitrobenzene	4.64 B	120 DR 4.64	
$C_6H_4ClNO_2$	*m*-Chloronitrobenzene	3.73 B	120 DR 3.73	
$C_6H_4ClNO_2$	*p*-Chloronitrobenzene	2.83 B	120 DR 2.83	
$C_6H_4Cl_2$	*o*-Dichlorobenzene	2.50 B	194 DR 2.48 156 DT 2.52	120
$C_6H_4Cl_2$	*m*-Dichlorobenzene	1.72 C	120 DR 1.72	
$C_6H_4Cl_2$	*p*-Dichlorobenzene	0 S	120 DR 0	
C_6H_4FI	*p*-Iodofluorobenzene	0.89 D	156 DR 0.89	
$C_6H_4FNO_2$	*p*-Fluoronitrobenzene	2.87 B	156 DR 2.87	
$C_6H_4F_2$	*m*-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
$C_6H_4N_2O_4$	*p*-Dinitrobenzene	0	S	131	DT	0	
$C_6H_4O_2$	1,4-Cyclohexadienedione (*p*-benzoquinone).	0	S	131	DT	0	068
C_6H_5Br	Bromobenzene	1.70	B	097	DT	1.70	
				321	DT	1.70	
				156	DR	1.77	
C_6H_5Cl	Chlorobenzene	1.69	B	101	DT	1.71	156, 273, 539
				084	DT	1.70	
				194	DT	1.67	
				520	MW	1.78	
C_6H_5ClO	*o*-Chlorophenol		i	148	DR	(a)	
C_6H_5ClO	*p*-Chlorophenol	2.11	C	148	DR	2.11	
C_6H_5F	Fluorobenzene	1.60	C	101	DT	1.58	
				194	DR	1.60	
				395	MW	1.66	
C_6H_5I	Iodobenzene	1.70	C	156	DR	1.70	
				321	DT	1.71	
$C_6H_5NO_2$	Nitrobenzene	4.22	B	101	DT	4.22	
				084	DR	4.27	
C_6H_6	Benzene	0	S	084	DT	0	157, 112, 011, 336
				113	DT	0	
				074	DT	0	
$C_6H_6N_2O_2$	*p*-Aminonitrobenzene (*p*-nitroaniline)	x	Q				068, 080
C_6H_6O	Phenol	1.45	C	120	DR	1.45	
$C_6H_6O_2$	*p*-Dihydroxybenzene	x	Q				068
C_6H_7N	Aminobenzene (aniline)	1.53	C	120	DR	1.53	
C_6H_8	1,3-Cyclohexadiene	0.44	B	553	MW	0.437	
C_6H_8	1,5-Hexadiyne		i	559	DR	0.57[b,c]	
$C_6H_8N_2$	*o*-Diaminobenzene	1.53	Di	148	DR	1.53	
$C_6H_8N_2$	*m*-Diaminobenzene	1.81	Di	148	DR	1.81	
$C_6H_8N_2$	*p*-Diaminobenzene	1.53	Di	148	DR	1.53	
$C_6H_8O_2$	1,4-Cyclohexanedione	(1.4)	Qi	463	DR	1.41	
C_6H_{10}	Cyclohexene	0.55	D	121	DR	0.55	
C_6H_{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_6H_{10}	2-Methyl-1,3-pentadiene	0.65 D	164 DR 0.65	
C_6H_{10}	3-Methyl-1,3-pentadiene	0.63 Di	164 DR 0.63	
C_6H_{10}	3,3-Dimethyl-1-butyne	0.66 A	489 MW 0.661	
C_6H_{10}	2-Ethyl-1,3-butadiene	(0.45) Qi	164 DR 0.45	
C_6H_{10}	2,3-Dimethyl-1,3-butadiene	0.52 Di	159 DR 0.52	
$C_6H_{10}BrCl$	*trans*-1-Bromo-2-chlorocyclohexane	i	463 DR 2.19[a]	
$C_6H_{10}Br_2$	*trans*-1,2-Dibromocyclohexane	i	463 DR 2.00[a]	
$C_6H_{10}Cl_2$	*cis*-1e,2a-Dichlorocyclohexane	3.11 C	287 DR 3.11	
$C_6H_{10}Cl_2$	*trans*-1,2-Dichlorocyclohexane	i	287 DR 2.31[a] 463 DR 2.29[a]	
$C_6H_{10}O_3$	Ethyl acetoacetate	i	082 DR 2.98[b]	
$C_6H_{12}N_2$	Diisopropylidene hydrazine (dimethyl ketazine).	1.53 Bi	151 DT 1.53	
$C_6H_{12}O_2$	Pentyl formate (n-amyl formate)	1.90 Ci	066 DT 1.90	
$C_6H_{12}O_3$	2,4,6-Trimethyl-1,3,5-trioxane (paraldehyde).	1.43 C	212 DT 1.43	
C_6H_{14}	Hexane	$\leqslant$0.1 Di	090 DT ≈ 0 098 DR ≈ 0	
$C_6H_{14}O$	Dipropyl ether	1.21 Ci	119 DT 1.21 062 DR 1.30	034
$C_6H_{14}O$	Diiospropyl ether	1.13 Di	251 DT 1.13	
$C_6H_{14}O_2$	1,1-Diethoxyethane	i	110 DR ([c])	
$C_6H_{15}N$	Triethyl amine	0.66 Ci	206 DT 0.66	052
$C_6H_{18}OSi_2$	Bis(trimethylsilyl) ether	(0.66) Qi	318 DR 0.66	
$C_7H_4ClF_3$	*o*-Chloro(trifluoromethyl)benzene	3.46 B	273 DR 3.46	
$C_7H_4ClF_3$	*p*-Chloro(trifluoromethyl)benzene	1.58 C	273 DR 1.58	
$C_7H_4N_2O_2$	*p*-Cyanonitrobenzene	(0) Q	131 DT ≈ 0	
$C_7H_5F_3$	(Trifluoromethyl)benzene	2.86 B	273 DR 2.86	
C_7H_5N	Cyanobenzene (benzonitrile)	4.18 B	299 MW 4.18[d] 084 DR 4.42	
C_7H_7Cl	*o*-Chlorotoluene	1.56 C	273 DR 1.56	
C_7H_7Cl	*p*-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_7H_7F	*o*-Fluorotoluene	1.37 C	194 DR 1.37	
C_7H_7F	*m*-Fluorotoluene	1.86 C	194 DR 1.86	
C_7H_7F	*p*-Fluorotoluene	2.00 C	194 DR 2.00	
$C_7H_7NO_3$	*o*-Nitro(methoxy)benzene	4.83 Bi	120 DR 4.83	
$C_7H_7NO_3$	*m*-Nitro(methoxy)benzene	4.55 Bi	120 DR 4.55	
$C_7H_7NO_3$	*p*-Nitro(methoxy)benzene	5.26 B	120 DR 5.26	
C_7H_8	1,3,5-Cycloheptatriene	0.25 C	554 MW 0.25	
C_7H_8	Toluene	0.36 C	142 DT 0.36 074 DT 0.36	
C_7H_8O	Phenylmethanol (benzyl alcohol)	1.71 C	288 DR 1.71	
C_7H_8O	Methoxybenzene (anisole)	1.38 C	120 DR 1.38	
C_7H_9NO	*o*-Amino(methoxy)benzene	1.61 Ci	148 DR 1.61	
C_7H_{10}	1,6-Heptadiyne	i	559 DR 0.81[a,b]	
C_7H_{12}	1-Heptyne	0.86 i	136 DR 0.87 559 DR 0.85[b]	
C_7H_{14}	Methylcyclohexane	(0) Qi	142 DT ≈0	
$C_7H_{14}O$	Methoxycyclohexane	1.35 Di	120 DR 1.35	
$C_7H_{14}O_2$	Pentyl acetate (*n*-amyl acetate)	1.75 Ci	066 DT 1.75	
$C_7H_{15}Br$	1-Bromoheptane	2.16 Ci	105 DR 2.16	
C_7H_{16}	Heptane	≤0.1 Di	098 DT ≈0 090 DT ≈0	112, 020
$C_8H_4N_2$	*p*-Dicyanobenzene	0 S	131 DT 0	
C_8H_8	Styrene	(0) Q	164 DR ≈0	
C_8H_8O	Acetylbenzene (acetophenone)	3.02 B	097 DT 3.02	
$C_8H_8O_2$	2,5-Dimethyl-1,4-cyclohexadienedione	0 S	131 DT 0	
$C_8H_9NO_2$	Methyl (*o*-aminophenyl)formate	x Q	....	018
$C_8H_9NO_2$	Methyl (*m*-aminophenyl)formate	x Q	....	018
$C_8H_9NO_2$	Methyl (*p*-aminophenyl)formate	x Q	....	018
C_8H_{10}	Ethylbenzene	0.59 C	142 DT 0.59	
C_8H_{10}	*o*-Xylene	0.62 C	156 DR 0.62[c]	
C_8H_{10}	*p*-Xylene	0 S	156 DR 0	
$C_8H_{10}O$	Ethoxybenzene (phenetole)	1.45 Di	120 DR 1.45	
$C_8H_{11}N$	(Dimethylamino)benzene	1.68 D	120 DR 1.68	
C_8H_{12}	1,7-Octadiyne	i	559 DR 0.88[a,b]	
$C_8H_{12}O_2$	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
$C_8H_{12}O_2$	Ethyl 2,4-hexadienoate (ethyl sorbate).	(2.07) Qi	166 DR 2.07	
$C_8H_{14}O_4$	Diethyl butanedioate (diethyl succinate).	i	064 DR (a)	
C_8H_{16}	Ethylcyclohexane	(0) Q	142 DT ≈ 0	
C_8H_{18}	Octane	≤ 0.1 Di	157 DR ≈ 0	
$C_8H_{18}O$	Dibutyl ether	1.17 Ci	119 DT 1.17	
C_9H_7N	Quinoline	2.29 C	329 DR 2.29	
C_9H_7N	Isoquinoline	2.73 C	329 DR 2.73	
$C_9H_{10}O_2$	Ethyl phenylformate (ethyl benzoate)	2.00 Ci	097 DR 2.00	
C_9H_{12}	Isopropylbenzene	(0.79) Q	142 DR 0.79	
$C_9H_{12}O_8$	Tetrakis(methyl carboxylate)methane	x Q		068
C_9H_{14}	1,8-Nonadiyne	i	559 DR 1.09[b, c]	
C_9H_{18}	Isopropylcyclohexane	(0) Q	142 DT ≈ 0	
$C_{10}H_8$	Azulene	0.80 B	575 MW 0.796	
$C_{10}H_{14}$	*t*-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	
$C_{10}H_{20}$	*t*-Butylcyclohexane	(0) Q	142 DT ≈ 0	
$C_{11}H_{16}$	*p*-*t*-Butyltoluene	x Q		142
$C_{12}H_8Br_2O$	Bis(*p*-bromophenyl) ether	1.02 D	132 DR 1.02	
$C_{12}H_9BrO$	*p*-Bromophenoxybenzene	1.98 C	132 DR 1.98	
$C_{12}H_9NO_3$	*p*-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
$C_{13}H_{11}BrO$	*p*-Bromophenoxy-*p*-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(*p*-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
$C_{20}H_{28}O_8Th$	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	$v=0$	7.1195[a]	0.0006	537
	$v=1$	7.2069	0.0008	
	$v=2$	7.2964	0.0012	
	$v=3$	7.3865	0.0018	
$^{37}Cl^{6}Li$—Lithium chloride	$v=0$	7.1192[a]	0.0008	537
	$v=1$	7.2071	0.0012	
	$v=2$	7.2972	0.0014	
ClNa—Sodium chloride	$v=0$	9.002	0.004	473a
	$v=1$	9.060	0.004	
	$v=2$	9.119	0.004	
CsF—Cesium fluoride	$v=0$	7.8750[b]	0.0002	341
	$v=1$	7.9472	0.0002	
$^{19}F^{6}Li$—Lithium fluoride	$v=0$	6.3276[c]	0.0001	527
	$v=1$	6.4151	0.0001	
	$v=2$	6.5034	0.0001	
	$v=3$	6.5933	0.0001	
FNa—Sodium fluoride	$v=0$	8.1558	0.0001	536
	$v=1$	8.2209	0.0001	
	$v=2$	8.2867	0.0001	
FRb—Rubidium fluoride	$v=0$	8.5465	0.0002	591
	$v=1$	8.6135	0.0002	
	$v=2$	8.6810	0.0002	
FTl—Thallium fluoride	$v=0$	4.2282	0.0001	397
	$v=1$	4.2971	0.0001	
	$v=2$	4.3665	0.0004	
HLi—Lithium hydride	$v=0$	5.882	0.003	442
	$v=1$	5.990	0.003	
$^{127}I^{6}Li$—Lithium iodide	$v=0$	7.4285	0.0002	552
	$v=1$	7.5120	0.0002	
OSr—Strontium oxide	$v=0$	8.900	0.003	562
	$v=1$	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.

Compound	Vibrational state	Dipole moment (debyes)	Precision (debyes)	References
O_2S—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_2H_2O—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 NH_3 (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	$^{79}\mathrm{Br}^{6}\mathrm{Li}$	7.2680[a]	0.0001	535
	$^{81}\mathrm{Br}^{6}\mathrm{Li}$	7.2678	0.0001	
	$^{79}\mathrm{Br}^{6}\mathrm{Li}$	7.2680	0.0002	591
	$^{79}\mathrm{Br}^{7}\mathrm{Li}$	7.2648	0.0002	
Lithium chloride	$^{35}\mathrm{Cl}^{6}\mathrm{Li}$	7.1195[a]	0.0006	537
	$^{37}\mathrm{Cl}^{6}\mathrm{Li}$	7.1192	0.0008	
Lithium fluoride	$^{19}\mathrm{F}^{6}\mathrm{Li}$	6.3275	0.0002	591
	$^{19}\mathrm{F}^{7}\mathrm{Li}$	6.3248	0.0002	
Thallium fluoride	$^{19}\mathrm{F}^{205}\mathrm{Tl}$	4.2282[b]	0.000001	397
	$^{19}\mathrm{F}^{203}\mathrm{Tl}$	4.2282	0.000001	
Lithium hydride	$^{1}\mathrm{H}^{6}\mathrm{Li}$	5.884	0.003	442
	$^{1}\mathrm{H}^{7}\mathrm{Li}$	5.882	0.003	
Carbon compounds:				
Trifluoromethane	$^{12}\mathrm{C}^{1}\mathrm{H}^{19}\mathrm{F}_3$	1.6460	0.001	587
	$^{12}\mathrm{C}^{2}\mathrm{H}^{19}\mathrm{F}_3$	1.6470[c]	0.001	
Fluoromethane	$^{12}\mathrm{C}^{1}\mathrm{H}_3{}^{19}\mathrm{F}$	1.8471	0.001	587
	$^{12}\mathrm{C}^{2}\mathrm{H}_3{}^{19}\mathrm{F}$	1.8583	0.001	
Methyl germane	$^{12}\mathrm{C}^{1}\mathrm{H}_3{}^{70}\mathrm{Ge}^{1}\mathrm{H}_3$	0.6425	0.001	587
	$^{12}\mathrm{C}^{1}\mathrm{H}_3{}^{74}\mathrm{Ge}^{1}\mathrm{H}_3$	0.6420	0.001	
	$^{12}\mathrm{C}^{1}\mathrm{H}_3{}^{70}\mathrm{Ge}^{2}\mathrm{H}_3$	0.6295	0.001	
	$^{12}\mathrm{C}^{1}\mathrm{H}_3{}^{74}\mathrm{Ge}^{2}\mathrm{H}_3$	0.6298	0.001	
	$^{12}\mathrm{C}^{2}\mathrm{H}_3{}^{70}\mathrm{Ge}^{1}\mathrm{H}_3$	0.6548	0.001	
	$^{12}\mathrm{C}^{2}\mathrm{H}_3{}^{74}\mathrm{Ge}^{1}\mathrm{H}_3$	0.6539	0.001	
Methyl silane	$^{12}\mathrm{C}^{1}\mathrm{H}_3{}^{28}\mathrm{Si}^{1}\mathrm{H}_3$	0.7351	0.001	587
	$^{12}\mathrm{C}^{1}\mathrm{H}_3{}^{28}\mathrm{Si}^{2}\mathrm{H}_3$	0.7236	0.001	
1,1-Difluoroethylene	$^{1}\mathrm{H}_2{}^{12}\mathrm{C}^{12}\mathrm{C}^{19}\mathrm{F}_2$	1.385	0.001	587
	$^{2}\mathrm{H}_2{}^{12}\mathrm{C}^{12}\mathrm{C}^{19}\mathrm{F}_2$	1.391	0.001	

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

Compound	Isotopic species	Dipole moment (debyes)	Precision (debyes)	Reference
Propyne	$^{12}C^{1}H_3{}^{12}C^{12}C^{1}H$	0.781	0.001	587
	$^{12}C^{1}H_3{}^{12}C^{12}C^{2}H$	0.768	0.001	
	$^{12}C^{2}H_3{}^{12}C^{12}C^{1}H$	0.784	0.001	
	$^{12}C^{2}H_3{}^{12}C^{12}C^{2}H$	0.772	0.001	
Propane	$^{12}C^{1}H_3{}^{12}C^{1}H_2{}^{12}C^{1}H_3$	0.0848	0.001	
	$^{12}C^{1}H_3{}^{12}C^{2}H_2{}^{12}C^{1}H_3$	0.0948	0.001	
	$^{12}C^{2}H_3{}^{12}C^{1}H_2{}^{12}C^{2}H_3$	0.0758	0.001	
2-Methylpropane	$(^{12}C^{1}H_3)_3{}^{12}C^{1}H$	0.1320	0.0006	432
	$(^{12}C^{1}H_3)_3{}^{12}C^{2}H$	0.1406	0.0006	

[a] See also appendix I.

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

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

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