double (**) asterisks stand for the values of $\mu_1$ and $\mu_2$, respectively. In all the other cases, the $\mu$'s listed are attributed to the molecule with the dominant isotopic composition and a non-excited electronic-vibration state.

Key information about the experimental methods of dipole moment measurement and accuracy estimation is given in [15.1.1–5].

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**Table 15.1.** Dipole moments of molecules

| Molecule or radical | Ground state dipole moment $\mu$ [debye] | Molecule or radical | Ground state dipole moment $\mu$ [debye] |
|---|---|---|---|
| Diatomic molecules | | | |
| AgCl | 6.1 (*B*) | ClF | 0.888 (*A*) |
| AgF | 6.2 (*C*) | ClO | 1.24 (*B*) |
| AlF | 1.53 (*B*) | CsBr | 10.8 (*A*) |
| BF | 0.5 (*D*) | CsCl | 10.387 (*A*) |
| BH | 1.3 (*D*) | | 10.445* (*A*) |
| BaO ($X^1\Sigma^+$) | 7.955 (*A*) | | 10.503** (*A*) |
| | 7.997* (*A*) | CsF | 7.883 (*A*) |
| | 8.039 ** (*A*) | | 7.953* (*A*) |
| ($A^1\Sigma^+$) | 2.2 ($v = 7$) (*B*) | | 8.024** (*A*) |
| BaS | 10.86 (*A*) | CsI | 11.7 (*A*) |
| | 10.88* (*A*) | CuF | 5.8 (*C*) |
| | 10.91** (*A*) | FO | 0.0043 (*C*) |
| BrCl | 0.519 (*A*) | | 0.027* (*C*) |
| BrF | 1.3 (*D*) | GaF | 2.4 (*C*) |
| BrO | 1.76 (*A*) | GeO | 3.282 (*A*) |
| CF | 0.65 (*D*) | | 3.303* (*A*) |
| CH | 1.45 (*C*) | | 3.324** (*A*) |
| CN | 1.4 (*D*) | GeS | 2.00 (*B*) |
| CO | 0.1098 (*A*) | GeSe | 1.65 (*A*) |
| CS | 1.97 (*A*) | GeTe | 1.06 (*B*) |
| CSe | 2.0 (*B*) | $^1H^2H$ | $5.5 \cdot 10^{-4}$ (*B*) |
| CaBr | 4.36 (*A*) | $^1H^2H^+$ | 0.87 (*B*) |
| CaCl | 4.26 (*A*) | HBr | 0.827 (*A*) |
| CaF | 3.1 (*B*) | $^2$HBr | 0.823 (*A*) |

**Table 15.1** (continued)

| Molecule or radical | Groun mome |
|---|---|
| HCl | 1.108 |
| | 1.139 |
| | 1.168 |
| $^2$HCl | 1.103 |
| | 1.126 |
| HF | 1.826 |
| $^2$HF | 1.819 |
| HI | 0.448 |
| $^2$HI | 0.44 ( |
| IBr | 0.74 ( |
| ICl | 1.24 ( |
| IO | 2.45 ( |
| InCl | 3.8 (*B* |
| InF | 3.4 (*B* |
| KBr | 10.628 |
| | 10.679 |
| | 10.729 |
| KCl | 10.269 |
| | 10.329 |
| | 10.388 |
| KF | 8.593 |
| | 8.661 |
| | 8.731 |
| KI | 10.8 (*A* |
| $^6$LiBr | 7.268 |
| | 7.352* |
| | 7.438* |
| $^7$LiBr | 7.265 |
| $^6$LiCl | 7.129 |
| | 7.217* |
| | 7.306* |
| $^7$LiCl | 7.129 |
| | 7.216* |
| | 7.305* |
| $^7$LiF | 6.325 |
| | 6.407* |
| | 6.491* |
| $^7$LiH ($X^1\Sigma^+$) | 5.882 |
| | 5.990* |
| | 6.098* |
| ($A^1\Sigma^+$) | 1.9* ( |
| | 1.5** ( |
| $^7$Li$^2$H | 5.868 ( |
| $^6$LiI | 7.428 ( |
| | 7.512* |
| $^7$LiK | 3.4 (*B* |
| $^7$LiNa | 0.46 (*I* |
| $^7$LiO | 6.8 (*B* |

$u_2$, respectively. In all the
lecule with the dominant
vibration state.
ds of dipole moment mea-
.1–5].

*its*, Vol. 2 (Rahara Enterprises,

*k of Dipole Moments*, 3rd ed.

ed Values of Electric Dipole
Ref. Data Ser. Nat. Bur. Stand.

*cular Structure IV. Constants of*
rk 1979)
in *Molecular Constants*, ed. by
(Springer, Berlin, Heidelberg,

| | Ground state dipole moment $\mu$ [debye] |
|---|---|
| | 0.888 (*A*) |
| | 1.24 (*B*) |
| | 10.8 (*A*) |
| | 10.387 (*A*) |
| | 10.445* (*A*) |
| | 10.503** (*A*) |
| | 7.883 (*A*) |
| | 7.953* (*A*) |
| | 8.024** (*A*) |
| | 11.7 (*A*) |
| | 5.8 (*C*) |
| | 0.0043 (*C*) |
| | 0.027* (*C*) |
| | 2.4 (*C*) |
| | 3.282 (*A*) |
| | 3.303* (*A*) |
| | 3.324** (*A*) |
| | 2.00 (*B*) |
| | 1.65 (*A*) |
| | 1.06 (*B*) |
| | $5.5 \cdot 10^{-4}$ (*B*) |
| | 0.87 (*B*) |
| | 0.827 (*A*) |
| | 0.823 (*A*) |



**Table 15.1** (continued)

| Molecule or radical | Ground state dipole moment $\mu$ [debye] |
|---|---|
| HCl | 1.108 (*A*) |
| | 1.139* (*A*) |
| | 1.168** (*A*) |
| $^2$HCl | 1.103 (*A*) |
| | 1.126* (*A*) |
| HF | 1.826 (*A*) |
| $^2$HF | 1.819 (*A*) |
| HI | 0.448 (*A*) |
| $^2$HI | 0.44 (*C*) |
| IBr | 0.74 (*B*) |
| ICl | 1.24 (*C*) |
| IO | 2.45 (*C*) |
| InCl | 3.8 (*B*) |
| InF | 3.4 (*B*) |
| KBr | 10.628 (*A*) |
| | 10.679* (*A*) |
| | 10.729** (*A*) |
| KCl | 10.269 (*A*) |
| | 10.329* (*A*) |
| | 10.388** (*A*) |
| KF | 8.593 (*A*) |
| | 8.661* (*A*) |
| | 8.731** (*A*) |
| KI | 10.8 (*A*) |
| $^6$LiBr | 7.268 (*A*) |
| | 7.352* (*A*) |
| | 7.438** (*A*) |
| $^7$LiBr | 7.265 (*A*) |
| $^6$LiCl | 7.129 (*A*) |
| | 7.217* (*A*) |
| | 7.306** (*A*) |
| $^7$LiCl | 7.129 (*A*) |
| | 7.216* (*A*) |
| | 7.305** (*A*) |
| $^7$LiF | 6.325 (*A*) |
| | 6.407* (*A*) |
| | 6.491** (*A*) |
| $^7$LiH ($X^1\Sigma^+$) | 5.882 (*A*) |
| | 5.990* (*A*) |
| | 6.098** (*A*) |
| ($A^1\Sigma^+$) | 1.9* (*C*) |
| | 1.5** (*C*) |
| $^7$Li$^2$H | 5.868 (*A*) |
| $^6$LiI | 7.428 (*A*) |
| | 7.512* (*A*) |
| $^7$LiK | 3.4 (*B*) |
| $^7$LiNa | 0.46 (*B*) |
| $^7$LiO | 6.8 (*B*) |
| $^7$LiRb | 4.0 (*B*) |
| NH ($a^1\Delta$) | 1.5 (*C*) |
| ($A^3\Pi$) | 1.3 (*C*) |
| ($c^1\Pi$) | 1.7 (*C*) |
| NO ($^2\Pi_{1/2}$) | 0.157 (*A*) |
| | 0.142* (*A*) |
| NS ($^2\Pi_{1/2}$) | 1.8 (*C*) |
| NaBr | 9.118 (*A*) |
| | 9.171* (*A*) |
| NaCl | 9.001 (*A*) |
| | 9.061* (*A*) |
| | 9.121** (*A*) |
| NaCs | 4.7 (*B*) |
| NaF | 8.156 (*A*) |
| | 8.221* (*A*) |
| | 8.287** (*A*) |
| NaI | 9,236 (*A*) |
| | 9.286* (*A*) |
| NaH | 6.4 (*C*) |
| NaK | 2.67 (*A*) |
| NaRb | 3.1 (*C*) |
| OH ($X^2\Pi_i$) | 1.655 (*A*) |
| ($A^2\Sigma^+$) | 1.98 (*B*) |
| O$^2$H ($X^2\Pi_i$) | 1.653 (*A*) |
| ($A^2\Sigma^+$) | 2.16 (*B*) |
| PN | 2.747 (*A*) |
| | 2.738* (*A*) |
| | 2.730** (*A*) |
| PbO | 4.6 (*B*) |
| PbS | 3.6 (*C*) |
| PbSe | 3.3 (*B*) |
| PbTe | 2.7 (*B*) |
| RbBr | 10.9 (*A*) |
| RbCl | 10.510 (*A*) |
| | 10.564* (*A*) |
| | 10.618** (*A*) |
| RbF | 8.546 (*A*) |
| | 8.613* (*A*) |
| | 8.681** (*A*) |
| RbI | 11.5 (*A*) |
| SF | 0.79 (*B*) |
| SH | 0.758 (*A*) |
| S$^2$H | 0.757 (*A*) |
| SO ($X^3\Sigma^-$) | 1.55 (*B*) |
| ($a^1\Delta$) | 1.32 (*B*) |
| SeF | 1.5 (*C*) |
| SeH | 0.50 (*C*) |
| Se$^2$H | 0.48 (*B*) |

**Table 15.1** (continued)

| Molecule or radical | Ground state dipole moment $\mu$ [debye] |
|---|---|
| SeO ($a\,^1\Delta$) | 2.01 (*B*) |
| SiH | 5.9 (*B*) |
| SiO | 3.098 (*A*) |
| | 3.118* (*A*) |
| | 3.137** (*A*) |
| SiS | 1.7 (*C*) |
| SnO | 4.32 (*B*) |
| SnS | 3.18 (*A*) |
| | 3.20* (*A*) |
| SnSe | 2.82 (*B*) |
| SnTe | 2.19 (*B*) |
| SrF | 3.50 (*A*) |
| | 3.55* (*A*) |
| SrO | 8.90 (*A*) |
| | 8.87* (*A*) |
| | 8.85** (*A*) |
| TlBr | 4.49 (*B*) |
| TlCl | 4.543 (*A*) |
| | 4.598* (*A*) |
| | 4.654** (*A*) |
| TlF | 4.228 (*A*) |
| | 4.297* (*A*) |
| | 4.366** (*A*) |
| TlI | 4.61 (*B*) |
| Triatomic molecules | |
| $CF_2$ | 0.46 (*B*) |
| $Cl_2O$ | 1.7 (*C*) |
| $ClO_2$ | 1.78 (*A*) |
| CsOH | 7.01 (*A*) |
| FCN | 2.17 (*B*) |
| $F_2O$ | 0.297 (*A*) |
| $F_2Si$ | 1.23 (*B*) |
| HCN | 2.98 (*A*) |
| $H_2O$ | 1.8473 (*A*) |
| $^2H_2O$ | 1.86 (*B*) |
| $H_2S$ | 0.978 (*A*) |
| $H_2Se$ | 0.24 (*C*) |
| HOCl | 1.3 (*D*) |
| $HgBr_2$ | 0 (*S*) |
| $N_2O$ | 0.1608 (*A*) |
| NOF | 1.81 (*B*) |
| $NO_2$ | 0.32 (*B*) |
| $^{15}NO_2$ | 0.29 (*C*) |
| NSCl | 1.87 (*B*) |
| NSF | 1.90 (*A*) |
| OCS | 0.715 (*A*) |
| ONBr | 1.8 (*C*) |
| ONCl | 1.86 (*B*) |
| $O_3$ | 0.534 (*B*) |
| SCTe | 0.17 (*B*) |
| $SF_2$ | 1.0 (*C*) |
| $SO_2$ | 1.633 (*A*) |
| $S_2F$ | 1.03 (*C*) |
| $S_2O$ | 1.47 (*B*) |
| $SiF_2$ | 1.23 (*B*) |
| Four-atomic molecules | |
| $BBr_3$ | 0 (*S*) |
| $BCl_3$ | 0 (*S*) |
| $BF_3$ | 0 (*S*) |
| $C_2H_2$ | 0 (*S*) |
| CHFO | 2.35 (*A*) |
| $CH_2O$ | 2.33 (*A*) |
| $COCl_2$ | 1.17 (*A*) |
| $ClF_3$ | 0.6 (*C*) |
| $F_2O_2$ | 1.44 (*B*) |
| $FeCl_3$ | 1.3 (*C*) |
| $HBF_2$ | 0.97 (*B*) |
| HCNO | 3.1 (*C*) |
| $H_2O_2$ | 2.2 (*C*) |
| $HNO_2$ (cis-) | 1.42 (*A*) |
| (trans-) | 1.86 (*A*) |
| HNSO | 0.911 (*A*) |
| $NF_3$ | 0.24 (*C*) |
| $NFO_2$ | 0.47 (*B*) |
| $NHF_2$ | 1.93 (*A*) |
| $N^2HF_2$ | 1.93 (*B*) |
| $NH_3$ | 1.47 (*A*) |
| $^{15}NH_3$ | 1.26 (*B*) |
| $N_2F_2$ | 0.16 (*C*) |
| $N_3H$ | 0.84 (*A*) |
| $NO_2Cl$ | 0.53 (*A*) |
| $PCl_3$ | 0.56 (*C*) |
| $PH_3$ | 0.574 (*A*) |
| $SOCl_2$ | 1.45 (*B*) |
| $SOF_2$ | 1.62 (*A*) |
| $SO_2F$ | 0.23 (*B*) |
| $SO_3$ | 0 (*S*) |
| $S_2F_2$ | 1.4 (*C*) |
| Five-atomic molecules | |
| $B_2O_3$ | 3.5 (*C*) |
| $CCl_4$ | 0 (*S*) |
| $CF_3Cl$ | 0.50 (*A*) |
| $CH_3Br$ | 1.84 (*B*) |
| $CH_3Cl$ | 1.892 (*A*) |
| $CH_3F$ | 1.847 (*A*) |

**Table 15.1** (continued)

| Molecule or radical | Ground st moment $\mu$ |
|---|---|
| $CH_4$ | $5.4 \cdot 10^{-4}$ |
| $CH_2{}^2H_2$ | 0.014 (*C*) |
| $CH_3I$ | 1.62 (*B*) |
| $CH_2O_2$ | 1.41 (*A*) |
| $FClO_3$ | 0.023 (*D*) |
| $GeH_3Br$ | 2.00 (*A*) |
| $HNO_3$ | 2.17 (*A*) |
| $KNO_3$ | 1.6 (*C*) |
| $N_2O_3$ | 2.12 (*A*) |
| $NSF_3$ | 1.91 (*B*) |
| $POF_3$ | 1.73 (*B*) |
| $PSF_3$ | 0.63 (*C*) |
| $SF_4$ | 0.632 (*A*) |
| $SO_2F_2$ | 1.12 (*B*) |
| $SeF_4$ | 1.78 (*B*) |
| $SrCO_3$ | 1.9 (*C*) |

## 15.2 Molecular Pola

The electric dipole polari
to (5.2). Here we give th
gas-phase molecules. Thi

$$\bar{\alpha}_{av} = (\alpha_1 + \alpha_2 + \alpha_3)$$

where $\alpha_{1,2,3}$ are the comp
the principal axes.

The numerical data
[15.2.1–6], in which the
are also discussed. The
classes (see the Introduct
bility, we made use of th

### References


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(Wiley, New York 196
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15.2.3 N.J.Bridge, A.D.Bucki
15.2.4 J.Applequist, J.R.Carl,
15.2.5 R.W.Molof, T.M.Mille
1816 (1974) (alkali dim
15.2.6 J.Rychlewski: Mol. Phy

**Table 15.1** (continued)

| Molecule or radical | Ground state dipole moment $\mu$ [debye] | Molecule or radical | Ground state dipole moment $\mu$ [debye] |
|---|---|---|---|
| $CH_4$ | $5.4 \cdot 10^{-6}$ (*B*) | Six-atomic molecules | |
| $CH_2{}^2H_2$ | 0.014 (*C*) | $BrF_5$ | 1.5 (*D*) |
| $CH_3I$ | 1.62 (*B*) | $IF_5$ | 2.3 (*C*) |
| $CH_2O_2$ | 1.41 (*A*) | $N_2H_4$ | 1.7 (*C*) |
| $FClO_3$ | 0.023 (*D*) | $PF_5$ | 0 (*S*) |
| $GeH_3Br$ | 2.00 (*A*) | Larger polyatomic molecules | |
| $HNO_3$ | 2.17 (*A*) | $C_2H_4O$ | 2.7 (*B*) |
| $KNO_3$ | 1.6 (*C*) | $SF_6$ | 0 (*S*) |
| $N_2O_3$ | 2.12 (*A*) | $UF_6$ | 0 (*S*) |
| $NSF_3$ | 1.91 (*B*) | $C_2H_6$ | 0 (*S*) |
| $POF_3$ | 1.73 (*B*) | $C_2H_4O_2$ | 1.70 (*B*) |
| $PSF_3$ | 0.63 (*C*) | $C_2H_4OS$ | 3.72 (*B*) |
| $SF_4$ | 0.632 (*A*) | $C_3H_6$ | 0.366 (*A*) |
| $SO_2F_2$ | 1.12 (*B*) | $C_3H_8$ | 0.084 (*A*) |
| $SeF_4$ | 1.78 (*B*) | | |
| $SrCO_3$ | 1.9 (*C*) | | |

## 15.2 Molecular Polarizabilities

The electric dipole polarizability of a molecule is a tensor quantity according to (5.2). Here we give the average dipole polarizability $\bar{\alpha}_{av}$ for a number of gas-phase molecules. This is derived from the relation

$$\bar{\alpha}_{av} = (\alpha_1 + \alpha_2 + \alpha_3)/3 \,,$$

where $\alpha_{1,2,3}$ are the components of the dipole polarizability tensor reduced to the principal axes.

The numerical data contained in Table 15.2 are based mainly on [15.2.1–6], in which the methods of measuring the molecular polarizability are also discussed. The numerical values listed are grouped into accuracy classes (see the Introduction). To convert the measurement units of polarizability, we made use of the conversion factor $1\,a_0^3 = 0.1482\,\text{Å}^3$.

### References


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15.2.6 J.Rychlewski: Mol. Phys. **41**, 833 (1980) ($H_2$, HD, $D_2$)

**Table 15.2.** Average static polarizabilities $\bar{\alpha}_{av}$ of molecules

| Molecule | $\bar{\alpha}_{av}$ [Å$^3$] | [$a_0^3$] | Accuracy class |
|---|---|---|---|
| **Diatomic molecules** | | | |
| $Br_2$ | 6.5 | 44 | (*D*) |
| CO | 1.95 | 13.2 | (*B*) |
| $Cl_2$ | 4.6 | 31 | (*C*) |
| $Cs_2$ | 13 | 90 | (*C*) |
| $D_2$ | 0.793 | 5.348 | (*A*) |
| HBr | 3.6 | 24 | (*C*) |
| HCl | 2.6 | 18 | (*C*) |
| HD | 0.798 | 5.387 | (*A*) |
| $H_2$ | 0.803 | 5.417 | (*A*) |
| HF | 0.83 | 5.6 | (*C*) |
| HI | 5.3 | 36 | (*C*) |
| $K_2$ | 60 | 410 | (*C*) |
| $Li_2$ | 34 | 230 | (*C*) |
| LiNa | 40 | 270 | (*D*) |
| $N_2$ | 1.75 | 11.8 | (*A*) |
| NO | 1.7 | 12 | (*C*) |
| $Na_2$ | 30 | 200 | (*C*) |
| $O_2$ | 1.59 | 10.7 | (*A*) |
| $Rb_2$ | 70 | 460 | (*D*) |
| **Triatomic molecules** | | | |
| $CO_2$ | 2.6 | 18 | (*C*) |
| $CS_2$ | 8.7 | 59 | (*C*) |
| HCN | 2.6 | 17 | (*C*) |
| $H_2O$ | 1.45 | 9.8 | (*B*) |
| $H_2S$ | 3.7 | 25 | (*C*) |
| $N_2O$ | 3.0 | 20 | (*B*) |
| $NO_2$ | 3.0 | 20 | (*C*) |
| $SO_2$ | 3.8 | 26 | (*C*) |
| **Four-atomic molecules** | | | |
| $C_2H_2$ | 3.5 | 24 | (*D*) |
| $H_2CO$ | 2.5 | 17 | (*D*) |
| $NH_3$ | 2.22 | 15.0 | (*B*) |
| **Five-atomic molecules** | | | |
| $CCl_4$ | 10.4 | 70 | (*B*) |
| $CF_4$ | 2.9 | 19 | (*C*) |
| $CHBr_3$ | 11.8 | 80 | (*B*) |
| $CHCl_3$ | 8.4 | 57 | (*C*) |
| $CHF_3$ | 2.9 | 20 | (*C*) |
| $CH_2Br_2$ | 8.7 | 59 | (*C*) |
| $CH_2Cl_2$ | 6.7 | 45 | (*B*) |
| $CH_3Br$ | 5.6 | 38 | (*C*) |
| $CH_3Cl$ | 4.56 | 30.8 | (*B*) |
| $CH_3F$ | 2.6 | 18 | (*C*) |
| $CH_4$ | 2.56 | 17.3 | (*B*) |
| $CH_3I$ | 7.6 | 51 | (*C*) |
| $CH_2I_2$ | 12.9 | 87 | (*C*) |
| $CHI_3$ | 18.0 | 120 | (*C*) |
| **Larger polyatomic molecules** | | | |
| $C_2H_4$ | 4.2 | 28 | (*C*) |
| $CH_3OH$ | 3.3 | 22 | (*C*) |
| $(NO_2)_2$ | 6.6 | 45 | (*D*) |
| $(CH_2)_2O$ | 4.4 | 30 | (*D*) |
| $CH_3NH_2$ | 4.0 | 27 | (*D*) |
| $SF_6$ | 6.55 | 44.2 | (*A*) |
| $C_2H_6$ | 4.5 | 30 | (*C*) |
| $O(CH_2CH_2)O$ | 8.6 | 58 | (*D*) |
| $C_3H_6$ | 9.1 | 62 | (*D*) |
| $C_2H_5 \cdot OH$ | 5.1 | 34 | (*C*) |
| $CH_3 \cdot O \cdot CH_3$ | 5.2 | 35 | (*C*) |
| $C_3H_8$ | 6.28 | 42.3 | (*B*) |
| $C_6H_6$ | 10.4 | 70 | (*B*) |
| $C_3H_7 \cdot OH$ | 7.0 | 47 | (*C*) |
| $C(CH_3)_4$ | 10.2 | 69 | (*B*) |
| $C_6H_{12}$ | 11.0 | 74 | (*B*) |
| $C_6H_{11} \cdot OH$ | 11.5 | 78 | (*B*) |