ATOMIC AND MOLECULAR POLARIZABILITIES

Thomas M. Miller

The *polarizability* of an atom or molecule describes the response of the electron cloud to an external field. The atomic or molecular energy shift ΔW due to an external electric field E is proportional to E^2 for external fields which are weak compared to the internal electric fields between the nucleus and electron cloud. The *electric dipole polarizability* α is the constant of proportionality defined by $\Delta W = -\alpha E^2/2$. The induced electric dipole moment is αE. *Hyperpolarizabilities*, coefficients of higher powers of E, are less often required. Technically, the polarizability is a tensor quantity but for spherically symmetric charge distributions reduces to a single number. In any case, an *average polarizability* is usually adequate in calculations. Frequency-dependent or *dynamic polarizabilities* are needed for electric fields which vary in time, except for frequencies which are much lower than electron orbital frequencies, where *static polarizabilities* suffice.

Polarizabilities for atoms and molecules in excited states are found to be larger than for ground states and may be positive or negative. Molecular polarizabilities are very slightly temperature dependent since the size of the molecule depends on its rovibrational state. Only in the case of dihydrogen has this effect been studied enough to warrant consideration in Table 3.

Polarizabilities are normally expressed in cgs units of cm^3. Ground state polarizabilities are in the range of 10^{-24} cm^3 = 1 $Å^3$ and hence are often given in $Å^3$ units. Theorists tend to use atomic units of a_o^3 where a_o is the Bohr radius. The conversion is $\alpha(cm^3) = 0.148184 \times 10^{-24} \times \alpha(a_o^3)$. Polarizabilities are only recently encountered in SI units, $C\,m^2/V = J/(V/m)^2$. The conversion from cgs units to SI units is $\alpha(C\,m^2/V) = 4\pi\varepsilon_o \times 10^{-6}\ \alpha(cm^3)$, where ε_o is the permittivity of free space in SI units and the factor 10^{-6} simply converts cm^3 into m^3. Thus, $\alpha(C\,m^2/V) = 1.11265 \times 10^{-16} \times \alpha(cm^3)$. Persons measuring excited state polarizabilities by optical methods tend to use units of $MHz/(V/cm)^2$, where the energy shift, ΔW, is expressed in frequency units with a factor of h understood. The polarizability is $-2\,\Delta W/E^2$. The conversion into cgs units is $\alpha(cm^3) = 5.95531 \times 10^{-16} \times \alpha[MHz/(V/cm)^2]$.

The polarizability appears in many formulas for low-energy processes involving the valence electrons of atoms or molecules. These formulas are given below in cgs units: the polarizability α is in cm^3; masses m or μ are in grams; energies are in ergs; and electric charges are in esu, where $e = 4.8032 \times 10^{-10}$ esu. The symbol $\alpha(\nu)$ denotes a frequency (ν) dependent polarizability, where $\alpha(\nu)$ reduces to the static polarizability a for $\nu = 0$. For further information, see Bonin, K. D., and Kresin, V. V., *Electric Dipole Polarizabilities of Atoms, Molecules, and Clusters*, World Scientific, Sinapore, 1997; Bonin, K. D., and Kadar-Kallen, *Int. J. Mod. Phys. B*, 24, 3313, 1994; and Miller, T. M., and Bederson, B., *Advances in Atomic and Molecular Physics*, 13, 1, 1977, and Gould, H., and Miller, T. M., *Advances in Atomic, Molecular, and Optical Physics,* 51, 243, 2005. Details on polarizability-related interactions, especially in regard to hyperpolarizabilities and nonlinear optical phenomena, are given by Bogaard, M. P., and Orr, B. J., in P*hysical Chemistry, Series Two, Vol.2, Molecular Structure and Properties*, Buckingham, A. D., Ed., Butterworths, London, 1975, pp. 149-194. A tabulation of tensor and hyperpolarizabilities is included. The gas number density, n, in Table 1 is usually taken to be that of 1 atm at 0°C in reporting experimental data.

TABLE 1. Formulas Involving Polarizability

Description	Formula	Remarks
Lorentz-Lorenz relation	$\alpha(\nu) = \frac{3}{4\pi n}\left[\frac{\eta^2(\nu)-1}{\eta^2(\nu)+2}\right]$	For a gas of atoms or nonpolar molecules; the index of refraction is $\eta(\nu)$
Refraction by polar molecules	$\alpha(\nu) + \frac{d^2}{3kT} = \frac{3}{4\pi n}\left[\frac{\eta^2(\nu)-1}{\eta^2(\nu)+2}\right]$	The dipole moment is d, in esu·cm (= 10^{-18} D)
Dielectric constant (dimensionless)	$\kappa(\nu) = 1 + 4\pi n\ \ \alpha(\nu)$	From the Lorentz-Lorenz relation for the usual case of $\kappa(\nu) \approx 1$
Index of refraction (dimensionless)	$\eta(\nu) = 1 + 2\pi n\ \ \alpha(\nu)$	From $\eta^3(\nu) = \kappa(\nu)$
Diamagnetic susceptibility	$\chi_m = e^2\left(a_o N\alpha\right)^{1/2} / 4m_e c^2$	From the approximation that the static polarizability is given by the variational formula $\alpha = (4/9a_o)\Sigma(N_i r_i^2)^2$; N is the number of electrons, m_e is the electron mass; a crude approximation is $\chi_m = (E_i/4m_e c^2)\alpha$, where E_i is the ionization energy
Long-range electron- or ion-molecule interaction energy	$V(r) = -e^2\alpha / 2r^4$	The target molecule polarizability is α
Ion mobility in a gas	$\kappa = -13.87 / \left(\alpha\mu\right)^{1/2} cm^2 / V \cdot s$	This one formula is not in cgs units. Enter α in $Å^3$ or 10^{-24} cm^3 units and the reduced mass μ of the ion-molecule pair in amu. Classical limit; pure polarization potential
Langevin capture cross section	$\sigma(\nu_o) = \left(2\pi e / \nu_o\right)\left(\alpha / \mu\right)^{1/2}$	The relative velocity of approach for an ion-molecule pair is ν_o; the target molecular polarizability is α and the reduced mass of the ion-molecule pair is μ
Langevin reaction rate coefficient	$k = 2\pi e\left(\alpha / \mu\right)^{1/2}$	Collisional rate coefficient for an ion-molecule reaction
Rate coefficient for polar molecules	$k_d = 2\pi e\left[\left(\alpha / \mu\right)^{1/2} + cd\left(2 / \mu\pi kT\right)^{1/2}\right]$	The dipole moment of the neutral is d in esu cm; the number c is a "locking factor" that depends on α and d, and is between 0 and 1

Description	Formula	Remarks
Modified effective range cross section for electron-neutral scattering	$\sigma(k) = 4\pi A^2 + 32\pi^4 \; e^2\alpha A k / 3h^2 + \ldots$	Here, k is the electron momentum divided by $h/2\pi$, where h is Planck's constant; A is called the "scattering length"; the reduced mass is μ
van der Waals constant between two systems A, B	$C_6 = \frac{3}{2}\left[\frac{\alpha^{\mathrm{A}}\alpha^{\mathrm{B}}E^{\mathrm{A}}E^{\mathrm{B}}}{E^{\mathrm{A}}+E^{\mathrm{B}}}\right]$	For the interaction potential term $V_6(\mathrm{r}) = -C_6 r^6$; $E^{\mathrm{A,B}}$ represents average dipole transition energiesand $\alpha^{\mathrm{A,B}}$ the respective polarizabilities of A, B
Dipole-quadrupole constant between two systems A, B	$C_8 = \frac{15}{4}\left[\frac{\alpha^{\mathrm{A}}\alpha_{\mathrm{q}}{}^{\mathrm{B}}E^{\mathrm{A}}E_{\mathrm{q}}{}^{\mathrm{B}}}{E^{\mathrm{A}}+E_{\mathrm{q}}{}^{\mathrm{B}}}\right] + \frac{15}{4}\left[\frac{\alpha_{\mathrm{q}}{}^{\mathrm{A}}\alpha^{\mathrm{B}}E_{\mathrm{q}}{}^{\mathrm{A}}E^{\mathrm{B}}}{E_{\mathrm{q}}{}^{\mathrm{A}}+E^{\mathrm{B}}}\right]$	For the interaction potential term $V_8(\mathrm{r}) = -C_8 r^8$; $E_{\mathrm{q}}^{\mathrm{A,B}}$ represents average quadrupole transition energies and $\alpha_{\mathrm{q}}^{\mathrm{A,B}}$ are the respective quadrupole polarizabilities of A, B
van der Waals constant between an atom and a surface	$\mathrm{C}_3 = \frac{\alpha g E^{\mathrm{A}}E^{\mathrm{S}}}{8\left(E^{\mathrm{A}}+E^{\mathrm{S}}\right)}$	For an interaction potential $V_3(\mathrm{r}) = -C_3 r^3$; $E^{\mathrm{A,S}}$ are characteristic energies of the atom and surface; $g = 1$ for a free-electron metal and $g = (\varepsilon_\infty - 1)/(\varepsilon_\infty + 1)$ for an ionic crystal
Relationship between α(ν) and oscillator strengths	$\alpha(\nu) = \frac{e^2h^2}{4\pi^2 m_{\mathrm{e}}}\Sigma\frac{f_k}{E_k^2-(h\nu)^2}$	Here, f_k is the oscillator strength from the ground state to an excited state k, with excitation energy E_k. This formula is often used to estimate static polarizabilities (ν = 0)
Dynamic polarizability	$\alpha(\nu) = \frac{\alpha E_{\mathrm{r}}{}^2}{E_{\mathrm{r}}{}^2-(h\nu)^2}$	Approximate variation of the frequency-dependent polarizability α(ν) from ν = 0 up to the first dipole-allowed electronic transition, of energy E_t; the static dipole polarizability is α(0); infrared contributions ignored
Rayleigh scattering cross section	$\alpha(\nu) = \frac{8\pi}{9c^4}(2\pi\nu)^4 \times\left[3\alpha^2(\nu)+2\gamma^2(\nu)/3\right]$	The photon frequency is ν; the polarizability anisotropy (the difference between polarizabilities parallel and perpendicular to the molecular axis) is γ(ν)
Verdet constant	$V(\nu) = \frac{\nu n}{2m_{\mathrm{e}}c^2}\left[\frac{\mathrm{d}\alpha(\nu)}{\mathrm{d}\nu}\right]$	Defined from $\theta = V(\nu)B$, where θ is the angle of rotation of linearly polarized light through a medium of number density n, per unit length, for a longitudinal magnetic field strength B (Faraday effect)

TABLE 2. Static Average Electric Dipole Polarizabilities for Ground State Atoms (in Units of 10^{-24} cm^3)

Atomic number	Atom	Polarizability	Estimated accuracy (%)	Method	Ref.
1	H	0.666793	"exact"	calc	MB77
2	He	0.2050522	"exact"	calc	LJS04
		0.2050	0.1	index/diel	NB65/OC67
3	Li	24.33	0.7	beam	MJBTV06
4	Be	5.60	2	calc	MB77
5	B	3.03	2	calc	MB77
6	C	1.76	2	calc	MB77
7	N	1.10	2	calc/index	MB77
8	O	0.802	2	calc/index	MB77
9	F	0.557	2	calc	MB77
10	Ne	0.3956	0.1	diel	OC67
11	Na	24.11	0.12	inter-ferom	ESCHP94
12	Mg	10.6	2	calc	MB77
		11.1	5	calc	S71
		10.6	5	calc	BM02
13	Al	6.8	4.4	beam	MMD90
14	Si	5.38	2	calc	MB77
15	P	3.63	2	calc	MB77
16	S	2.90	2	calc	MB77
17	Cl	2.18	2	calc	MB77
18	Ar	1.6411	0.05	index/diel	NB65/OC67
19	K	43.4	2	beam	MB77
20	Ca	22.8	2	calc	MB77
		29.4	6	calc	BM02
		25.0	8	beam	MB77
21	Sc	17.8	25	calc	D84
22	Ti	14.6	25	calc	D84
23	V	12.4	25	calc	D84
24	Cr	11.6	25	calc	D84
25	Mn	9.4	25	calc	D84
26	Fe	8.4	25	calc	D84
27	Co	7.5	25	calc	D84
28	Ni	6.8	25	calc	D84
29	Cu	6.2	6	calc	BM02
		6.1	25	calc	D84
30	Zn	5.75	2	index	GHM96
		6.1	6	calc	BM02
		5.6	25	calc	D84
31	Ga	8.12	2	calc	MB77
32	Ge	6.07	2	calc	MB77
33	As	4.31	2	calc	MB77
34	Se	3.77	2	calc	MB77
35	Br	3.05	2	calc	MB77

Atomic number	Atom	Polarizability	Estimated accuracy (%)	Method	Ref.
36	Kr	2.4844	0.05	diel	OC67
37	Rb	47.3	2	beam	MB77
38	Sr	27.6	8	beam	MB77
		23.5	6	calc	BM02
39	Y	22.7	25	calc	D84
40	Zr	17.9	25	calc	D84
41	Nb	15.7	25	calc	D84
42	Mo	12.8	25	calc	D84
43	Tc	11.4	25	calc	D84
44	Ru	9.6	25	calc	D84
45	Rh	8.6	25	calc	D84
46	Pd	4.8	25	calc	D84
47	Ag	7.2	25	calc	D84
48	Cd	7.36	3	index	GH95
		7.4	6	calc	BM02
		7.2	25	calc	D84
49	In	10.2	12	beam	GMBSJ84
		9.1	25	calc	D84
50	Sn	7.7	25	calc	D84
51	Sb	6.6	25	calc	D84
52	Te	5.5	25	calc	D84
53	I	5.35	25	index	A56
		4.7	25	calc	D84
54	Xe	4.044	0.5	diel	MB77
55	Cs	59.42	0.13	beam	AG03
56	Ba	39.7	8	beam	MB77
57	La	31.1	25	calc	D84
58	Ce	29.6	25	calc	D84
59	Pr	28.2	25	calc	D84
60	Nd	31.4	25	calc	D84
61	Pm	30.1	25	calc	D84
62	Sm	28.8	25	calc	D84
63	Eu	27.7	25	calc	D84
64	Gd	23.5	25	calc	D84
65	Tb	25.5	25	calc	D84
66	Dy	24.5	25	calc	D84
67	Ho	23.6	25	calc	D84
68	Er	22.7	25	calc	D84
69	Tm	21.8	25	calc	D84
70	Yb	21.0	25	calc	D84
71	Lu	21.9	25	calc	D84
72	Hf	16.2	25	calc	D84
73	Ta	13.1	25	calc	D84
74	W	11.1	25	calc	D84
75	Re	9.7	25	calc	D84
76	Os	8.5	25	calc	D84
77	Ir	7.6	25	calc	D84
78	Pt	6.5	25	calc	D84
79	Au	5.8	25	calc	D84
80	Hg	5.02	1	index	GH96
		5.7	25	calc	D84
81	Tl	7.6	15	beam	NYU84
		7.5	25	calc	D84
82	Pb	6.8	25	calc	D84
83	Bi	7.4	25	calc	D84
84	Po	6.8	25	calc	D84
85	At	6.0	25	calc	D84
86	Rn	5.3	25	calc	D84
87	Fr	48.60	2	calc	LSMS05
		47.1	5	calc	DJSB99
88	Ra	38.3	25	calc	D84
89	Ac	32.1	25	calc	D84
90	Th	32.1	25	calc	D84
91	Pa	25.4	25	calc	D84
92	U	24.9	6	beam	KB94
93	Np	24.8	25	calc	D84
94	Pu	24.5	25	calc	D84
95	Am	23.3	25	calc	D84
96	Cm	23.0	25	calc	D84
97	Bk	22.7	25	calc	D84
98	Cf	20.5	25	calc	D84
99	Es	19.7	25	calc	D84
100	Fm	23.8	25	calc	D84
101	Md	18.2	25	calc	D84
102	No	17.5	25	calc	D84
119	ekafrancium	24.26	2	cal	LSMS05

[a] Methods: calc = calculated value; beam = atomic beam deflection technique; interferom = atomic beam interference; index = determination based on the measured index of refraction; diel = determination based on the measured dielectric constant.

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TABLE 3. Average Electric Dipole Polarizabilities for Ground State Diatomic Molecules (in Units of 10^{-24} cm^3)

Molecule	Polarizability	Ref.
Al_2	19	23
BH	3.32*	1
Br_2	7.02	2
CO	1.95	3
Cl_2	4.61	3
Cs_2	104	22
CsK	89	22
D_2 (v=0,J=0)	0.7921*	5
D_2 (293 K)	0.7954	6
DCl	2.84	2
F_2	1.38*	7
H_2 (v=0,J=0)	0.8023*	5
H_2 (293 K)	0.8045*	5
H_2 (293 K)	0.8042	6
H_2 (322 K)	0.8059	8
HBr	3.61	3
HCl	2.63	3
	2.77	2
HD (v=0,J=0)	0.7976*	5
HF	0.80	27
HI	5.44	3
	5.35	2
HgCl	7.4*	9
ICl	12.3	2
K_2	77	22
	72	21
Li_2	32.8	29
	34	22
LiCl	3.46*	10
LiF	10.8*	11
LiH	3.84*	12
	3.68*	13
	3.88*	14
N_2	1.7403	6,8
NO	1.70	2
Na_2	40	22
	38	21
NaK	51	22
NaLi	40	4
O_2	1.5812	6
Rb_2	79	22

TABLE 4. Average Electric Dipole Polarizabilities for Ground State Triatomic Molecules (in Units of 10^{-24} cm^3)

Molecule	Polarizability	Ref.
BeH_2	4.34*	14
CO_2	2.911	8
CS_2	8.74	3
	8.86	2
D_2O	1.26	2
H_2O	1.45	2
H_2S	3.782	3
	3.95	2
HCN	2.59	3
	2.46	2
$HgBr_2$	14.5	2
$HgCl_2$	11.6	2
HgI_2	19.1	2
Li_3	34.5	29
$LiNa_2$	61.2	30
Li_2Na	35.4	30
N_2O	3.03	8
NO_2	3.02	2†
Na_3	70	21
O_3	3.21	2
OCS	5.71	2
	5.2	15
SO_2	3.72	3
	4.28	2

TABLE 5. Average Electric Dipole Polarizabilities for Ground State Inorganic Polyatomic Molecules (Larger than Triatomic) (in Units of 10^{-24} cm^3)

Molecule	Polarizability	Ref.
$AsCl_3$	14.9	2
AsN_3	5.75	2
BCl_3	9.38	20
BF_3	3.31	2
$(BN_3)_2$	5.73	2
$(BH_2N)_3$	8.0	2†
ClF_3	6.32	2
$(CsBr)_2$	54.5	16
$(CsCl)_2$	42.4	16
$(CsF)_2$	28.4	16
$(CsI)_2$	51.8	16
Ga_nAs_m	n+m=4-30	28
$GeCl_4$	15.1	2
GeH_3Cl	6.7	2†
$(HgCl)_2$	14.7	9
K_n	n=2,5,7-9,11,20	21
$(KBr)_2$	42.0	16
$(KCl)_2$	32.1	16
$(KF)_2$	21.0	16
$(KI)_2$	36.3	16
Li_n	n=2-22	29
$(LiBr)_2$	18.9	16
$(LiCl)_2$	13.1	16
$(LiF)_2$	6.9	16
$(LiI)_2$	23.4	16
$LiNa_3$	75.6	30
Li_2Na_2	60.0	30
Li_3Na	54.8	30

Molecule	Polarizability	Ref.
ND_3	1.70	2
NF_3	3.62	2
NH_3	2.81	20
	2.10	2
	2.26	3
	2.22*	33
$(NO_2)_2$	6.69	2
Na_n	n=1-40	21
$(NaBr)_2$	26.8	16
$(NaCl)_2$	23.4	16
$(NaF)_2$	20.7	16
$(NaI)_2$	26.9	16
OsO_4	8.17	2
PCl_3	12.8	2
PF_5	6.10	2
PH_3	4.84	2
$(RbBr)_2$	48.2	16
$(RbCl)_2$	43.2	16
$(RbF)_2$	40.7	16
$(RbI)_2$	46.3	16
SF_6	6.54	8
$(SF_5)_2$	13.2	2
SO_3	4.84	2
SO_2Cl_2	10.5	2
SeF_6	7.33	2
SiF_4	5.45	2
SiH_4	5.44	2
$(SiH_3)_2$	11.1	2
$SiHCl_3$	10.7	2
SiH_2Cl_2	8.92	2
SiH_3Cl	7.02	2
$SnBr_4$	22.0	2
$SnCl_4$	18.0	2
	13.8	15
SnI_4	32.3	2
TeF_6	9.00	2
$TiCl_4$	16.4	2
UF_6	12.5	2

TABLE 6. Average Electric Dipole Polarizabilities for Ground State Hydrocarbon Molecules (in Units of 10^{-24} cm^3)

Molecule	Name	Polarizability	Ref.
CH_4	methane	2.593	8
C_2H_2	acetylene	3.33	3
		3.93	2
C_2H_4	ethylene	4.252	8
C_2H_6	ethane	4.47	3
		4.43	2
C_3H_4	propyne	6.18	2
C_3H_6	propene	6.26	2
	cyclopropane	5.66	2
C_3H_8	propane	6.29	3
		6.37	2
C_4H_6	1-butyne	7.41	2†
	1,3-butadiene	8.64	2
C_4H_8	1-butene	7.97	2
		8.52	2
	trans-2-butene	8.49	2
	2-methylpropene	8.29	2
C_4H_{10}	butane	8.20	2
	isobutane	8.14	27
C_5H_6	1,3-cyclopentadiene	8.64	2
C_5H_8	1-pentyne	9.12	2
	trans-1,3-pentadiene	10.0	2
	isoprene	9.99	2
C_5H_{10}	cyclopentane	9.15	18
	1-pentene	9.65	27
	2-pentene	9.84	27
C_5H_{12}	pentane	9.99	2
	neopentane	10.20	18
C_6H_6	benzene	10.0	25
		10.32	3
		10.74	2
C_6H_{10}	1-hexyne	10.9	2†
	2-ethyl-1,3-butadiene	11.8	2†
	3-methyl-1,3-pentadiene	11.8	2†
	2-methyl-1,3-pentadiene	12.1	2†
	2,3-dimethyl-1,3-butadiene	11.8	2†
	cyclohexene	10.7	2†
C_6H_{12}	cyclohexane	11.0	18
		10.87	15
	1-hexene	11.65	27
C_6H_{14}	hexane	11.9	2
C_7H_8	toluene	11.8	25
		12.26	15
		12.3	2
C_7H_{12}	1-heptyne	12.8	2†
C_7H_{14}	methylcyclohexane	13.1	2
	1-heptene	13.51	27
C_7H_{16}	heptane	13.61	2
C_8H_8	styrene	15.0	2
		14.41	27
C_8H_{10}	ethylbenzene	14.2	2
	o-xylene	14.9	2
		14.1	15
	p-xylene	13.7	25
		14.2	15
		14.9	2
	m-xylene	14.2	15
C_8H_{16}	ethylcyclohexane	15.9	2
C_8H_{18}	*n*-octane	15.9	2
	3-methylheptane	15.44	27
	2,2,4-trimethylpentane	15.44	27
C_9H_{10}	α- methylstyrene	16.05	27
C_9H_{12}	isopropylbenzene	16.0	2†
	1,3,5-trimethylbenzene	15.5	25
		16.14	27
C_9H_{18}	isopropylcyclohexane	17.2	2
C_9H_{20}	nonane	17.36	27
$C_{10}H_8$	naphthalene	16.5	17
		17.48	27
$C_{10}H_{14}$	durene	17.3	25
	tert- butylbenzene	17.2	25
		17.8	2†
$C_{10}H_{20}$	*tert*-butylcyclohexane	19.8	2
$C_{10}H_{22}$	decane	19.10	27
$C_{11}H_{10}$	α-methylnaphthalene	19.35	27
	β-methylnaphthalene	19.52	27

Molecule	Name	Polarizability	Ref.
$C_{11}H_{14}$	α,β,β-trimethylstyrene	19.64	27
$C_{11}H_{16}$	pentamethylbenzene	19.1	25
$C_{11}H_{24}$	undecane	21.03	27
$C_{12}H_{10}$	acenaphthene	20.61	27
$C_{12}H_{12}$	α-ethylnaphthalene	21.19	27
	β-ethylnaphthalene	21.36	27
$C_{12}H_{18}$	hexamethylbenzene	20.9	25
$C_{12}H_{26}$	dodecane	22.75	27
$C_{13}H_{10}$	fluorene	21.68	27
$C_{14}H_{10}$	anthracene	25.4	17
		25.93	27
	phenanthrene	36.8*	17
		24.70	27
$C_{14}H_{22}$	*p*-di-*tert*-butylbenzene	24.5	25
$C_{16}H_{10}$	pyrene	28.22	27
$C_{17}H_{12}$	2,3- benzfluorene	30.21	27
$C_{18}H_{12}$	naphthacene	32.27	27
	1,2- benzanthracene	32.86	27
	chrysene	33.06	27
	triphenylene	31.07	27
$C_{18}H_{30}$	1,3,5-tri-*tert*-butylbenzene	31.8	25
$C_{24}H_{12}$	coronene	42.50	27

TABLE 7. Average Electric Dipole Polarizabilities for Ground State Organic Halides (in Units of 10^{-24} cm^3)

Molecule	Name	Polarizability	Ref.
CBr_2F_2	dibromodifluoromethane	9.0	2†
$CClF_3$	chlorotrifluoromethane	5.72	20
		5.59	2
CCl_2F_2	dichlorodifluoromethane	7.93	20
		7.81	2
CCl_2O	phosgene	7.29	2
CCl_2S	thiophosgene	10.2	2
CCl_3F	trichlorofluoromethane	9.47	2
CCl_3NO_2	trichloronitromethane	10.8	2†
CCl_4	carbon tetrachloride	11.2	2
		10.5	3
CF_4	carbon tetrafluoride	3.838	8
CF_2O	carbonylfluoride	1.88*	17
$CHBr_3$	bromoform	11.8	27
$CHBrF_2$	bromodifluoromethane	5.7	2†
$CHClF_2$	chlorodifluoromethane	6.38	20
		5.91	2
$CHCl_2F$	dichlorofluoromethane	6.82	2
$CHCl_3$	chloroform	9.5	8
		8.23	27
CHF_3	fluoroform	3.52	20
		3.57	8
CHFO	fluoroformaldehyde	1.76*	17
CHI_3	iodoform	18.0	27
CH_2Br_2	dibromomethane	9.32	2
		8.68	27
CH_2ClNO_2	chloronitromethane	6.9	2†
CH_2Cl_2	dichloromethane	6.48	3
		7.93	2
CH_2I_2	diiodomethane	12.90	27
CH_3Br	bromomethane	5.87	20
		6.03	2
		5.55	15
CH_3Cl	chloromethane	5.35	20
		4.72	8
CH_3F	fluoromethane	2.97	8
CH_3I	iodomethane	7.97	2
C_2ClF_5	chloropentafluoroethane	6.3	2†
$C_2Cl_2F_4$	1,2-dichlorotetrafluoroethane	8.5	2†
C_2Cl_3N	trichloroacetonitrile	10.42	18
C_2F_6	hexafluoroethane	6.82	2
C_2HBr	bromoacetylene	7.39	2
C_2HCl	chloroacetylene	6.07	2
C_2HCl_3	trichloroethlyene	10.03	27
C_2HCl_5	pentachloroethane	14.0	2
$C_2H_2Cl_2$	1,1-dichloroethylene	7.83	27
	trans-dichloroethylene	8.15	27
	cis-dichloroethylene	8.03	27
$C_2H_2Cl_2F_2$	1,1-dichloro-2,2-difluoroethane	8.4	2†
$C_2H_2Cl_2O$	chloroacetyl chloride	8.92	2
$C_2H_2Cl_3F$	1,2,2-trichloro-1-fluoroethane	10.2	2†
$C_2H_2Cl_4$	1,1,2,2-tetrachloroethane	12.1	2†
C_2H_2ClN	chloroacetonitrile	6.10	18
$C_2H_2F_2$	1,1-difluoroethylene	5.01	20
C_2H_3Br	bromoethylene	7.59	2
C_2H_3Cl	chloroethylene	6.41	2
$C_2H_3ClF_2$	1-chloro-1,1-difluoroethane	8.05	2
C_2H_3ClO	acetyl chloride	6.62	2
$C_2H_3ClO_2$	methyl chloroformate	7.1	2†
$C_2H_3Cl_3$	1,1,1-trichloroethane	10.7	2
$C_2H_3F_3$	1,1,1-trifluoroethane	4.4	2†
C_2H_3I	iodoethylene	9.3	2†
C_2H_4BrCl	1-bromo-2-chloroethane	9.5	2†
$C_2H_4Br_2$	1,2-dibromoethane	10.7	2†
C_2H_4ClF	1-chloro-2-fluoroethane	6.5	2†
$C_2H_4ClNO_2$	1-chloro-1-nitroethane	10.9	2
$C_2H_4Cl_2$	1,1-dichloroethane	8.64	2
	1,2-dichloroethane	8.0	2†
C_2H_5Br	bromoethane	8.05	2
		7.28	27
C_2H_5Cl	chloroethane	7.27	20
		8.29	2
		6.4	15
C_2H_5ClO	2-chloroethanol	7.1	2†
		6.88	27
	chloromethyl methyl ether	7.1	2†
C_2H_5F	fluoroethane	4.96	2
C_2H_5I	iodoethane	10.0	2
$C_3H_4Cl_2$	dichloropropene	10.1	2†
C_3H_5Cl	chloropropene	8.3	2
C_3H_5ClO	chloroacetone	8.4	2†
$C_3H_5ClO_2$	ethyl chloroformate	9.0	2†
$C_3H_6ClNO_2$	1-chloro-1-nitropropane	10.4	2†
$C_3H_6Cl_2$	dichloropropane	10.9	2†
C_3H_7Br	1-bromopropane	9.4	2†
		9.07	27
	2-bromopropane	9.6	2†
C_3H_7Cl	chloropropane	10.0	2
C_3H_7ClO	β-chloroethyl methyl ether	8.71	27
	2-chloro-1-propanol	8.89	27
	3-chloro-1-propanol	8.84	27

Molecule	Name	Polarizability	Ref.
C_3H_7I	1-iodopropane	11.5	2†
C_4H_5Cl	4-chloro-1,2-butadiene	10.0	2†
C_4H_7Cl	1-chloro-2-methylpropene	10.8	2
$C_4H_7ClO_2$	2-chlorobutyric acid	10.87	27
	3-chlorobutyric acid	10.80	27
	4-chlorobutyric acid	10.69	27
$C_4H_8Cl_2$	1,4-dichlorobutane	12.0	2†
C_4H_9Br	bromobutane	13.9	2
		10.86	27
C_4H_9Cl	1-chlorobutane	11.3	2
	1-chloro-2-methylpropane	11.1	2
	2-chloro-2-methylpropane	12.5	2†
	2-chlorobutane	12.4	2
C_4H_9ClO	β-chloroethyl ethyl ether	10.56	27
	2-chloro-1-butanol	10.70	27
	3-chloro-1-butanol	10.38	27
C_4H_9I	1-iodobutane	13.3	2†
		12.65	27
$C_5H_9ClO_2$	methyl 2-chlorobutanoate	12.33	27
	methyl 3-chlorobutanoate	12.31	27
	methyl 4-chlorobutanoate	12.27	27
	2-chloropentanoic acid	12.69	27
	3-chloropentanoic acid	12.57	27
	4-chloropentanoic acid	12.53	27
$C_5H_{11}Br$	1-bromopentane	13.1	2†
$C_5H_{11}Cl$	1-chloropentane	12.0	2†
$C_5H_{11}F$	fluoropentane	9.95	27
C_6F_6	hexafluorobenzene	9.58	27
C_6HF_5	pentafluorobenzene	9.63	27
$C_6H_2Cl_2O_2$	2,5-dichloro-1,4-benzoquinone	18.4	2
$C_6H_2F_4$	1,2,3,4-tetrafluorobenzene	9.69	27
	1,2,4,5-tetrafluorobenzene	9.69	27
$C_6H_3F_3$	1,3,5-trifluorobenzene	9.74	27
C_6H_4BrF	*p*-bromofluorobenzene	13.4	2†
$C_6H_4ClNO_2$	chloronitrobenzene	14.6	2†
$C_6H_4Cl_2$	*o*-dichlorobenzene	14.17	27
	m-dichlorobenzene	14.23	27
	p-dichlorobenzene	14.20	27
C_6H_4FI	*p*-fluoroiodobenzene	15.5	2†
$C_6H_4FNO_2$	*p*-fluoronitrobenzene	12.8	2†
$C_6H_4F_2$	*o*-difluorobenzene	9.80	27
	m-difluorobenzene	10.3	2†
	p-difluorobenzene	9.80	27
C_6H_5Br	bromobenzene	14.7	2
		13.62	27
C_6H_5Cl	chlorobenzene	14.1	2
		12.3	15
C_6H_5ClO	chlorophenol	13.0	2†
C_6H_5F	fluorobenzene	10.3	2
C_6H_5I	iodobenzene	15.5	2†
$C_6H_{11}ClO_2$	ethyl 2-chlorobutanoate	14.16	27
	ethyl 3-chlorobutanoate	14.13	27
	ethyl 4-chlorobutanoate	14.11	27
$C_6H_{13}Br$	bromohexane	14.44	27
$C_6H_{13}F$	fluorohexane	11.80	27
C_7H_7Br	*p*-bromotoluene	14.80	27
C_7H_7Cl	*p*-chlorotoluene	13.70	27
C_7H_7F	*p*-fluorotoluene	11.70	27
C_7H_7I	*p*-iodotoluene	17.10	27
$C_7H_{15}Br$	1-bromoheptane	16.8	2†
		16.23	27
$C_7H_{15}F$	fluoroheptane	13.66	27
$C_8H_{17}Br$	bromooctane	18.02	27
$C_8H_{17}F$	fluorooctane	15.46	27
$C_9H_{19}Br$	bromononane	19.81	27
$C_9H_{19}F$	fluorononane	17.34	27
$C_{10}F_8$	octafluoronaphthalene	17.64	27
$C_{10}H_7Br$	α-bromonaphthalene	20.34	27
$C_{10}H_7Cl$	α-chloronaphthalene	19.30	27
	β-chloronaphthalene	19.58	27
$C_{10}H_7I$	α-iodonaphthalene	22.41	27
	β-iodonaphthalene	22.95	27
$C_{10}H_{21}Br$	bromodecane	21.60	27
$C_{10}H_{21}F$	fluorodecane	19.18	27
$C_{11}H_{23}F$	fluoroundecane	21.00	27
$C_{12}H_{25}Br$	bromododecane	25.18	27
$C_{12}H_{25}F$	fluorododecane	22.83	27
$C_{12}H_8Br_2O$	4,4'-dibromodiphenyl ether	27.8	2†
$C_{12}H_9BrO$	4-bromodiphenyl ether	24.2	2†
$C_{13}H_{11}BrO$	*p*-bromophenyl-*p*-tolyl ether	26.6	2†
$C_{14}H_9Br$	9-bromoanthracene	28.32	27
$C_{14}H_9Cl$	9-chloroanthracene	27.35	27
$C_{14}H_9F$	fluoranthracene	28.34	27
$C_{14}H_{29}F$	fluorotetradecane	26.57	27
$C_{16}H_{33}Br$	bromohexadecane	32.34	27
$C_{18}H_{37}Br$	bromooctadecane	35.92	27

TABLE 8. Static Average Electric Dipole Polarizabilities for Other Ground State Organic Molecules (in Units of 10^{-24} cm^3)

Molecule	Name	Polarizability	Ref.
CN_4O_8	tetranitromethane	15.3	2
CH_2O	formaldehyde	2.8	2†
		2.45	18
CH_2O_2	formic acid	3.4	2†
CH_3NO	formamide	4.2	2†
		4.08	18
CH_3NO_2	nitromethane	7.37	2
CH_4O	methanol	3.29	2
		3.23	15
		3.32	18
CH_5N	methyl amine	4.7	2
		4.01	19
		4.01*	33
C_2N_2	cyanogen	7.99	2
C_2H_2O	ketene	4.4	2†
C_2H_3N	acetonitrile	4.40	2†
		4.48	18
C_2H_4O	acetaldehyde	4.6	2†
		4.59	18
	ethylene oxide	4.43	18
$C_2H_4O_2$	acetic acid	5.1	2†
	methyl formate	5.05	27
$C_2H_4O_4$	formic acid dimer	12.7	2
C_2H_5NO	acetamide	5.67	18
	N-methyl formamide	5.91	18
$C_2H_5NO_2$	nitroethane	9.63	2
	ethyl nitrite	7.0	15
C_2H_6O	ethanol	5.41	2
		5.11	18
	methyl ether	5.29	20

Molecule	Name	Polarizability	Ref.
		5.84	2
		5.16	15
$C_2H_6O_2$	ethylene glycol	5.7	2†
		5.61	27
$C_2H_6O_2S$	dimethyl sulfone	7.3	2†
C_2H_6S	ethanethiol	7.41	2
C_2H_7N	ethyl amine	7.10	2
	dimethyl amine	6.37	2
		5.90*	33
$C_2H_8N_2$	ethylene diamine	7.2	2†
$C_3H_2N_2$	malononitrile	5.79	18
C_3H_3N	acrylonitrile	8.05	2
$C_3H_4N_2$	pyrazole	7.23	27
C_3H_4O	propenal	6.38	2†
C_3H_5N	propionitrile	6.70	2
		6.24	18
		6.27*	32
C_3H_6O	acetone	6.33	15
		6.4	2†
		6.39	18
	allyl alcohol	7.65	2
	propionaldehyde	6.50	2
$C_3H_6O_2$	propionic acid	6.9	2†
	ethyl formate	8.01	2
		6.88	27
	methyl acetate	6.94	2
		6.81	27
$C_3H_6O_3$	dimethyl carbonate	7.7	2†
C_3H_7NO	*N*-methyl acetamide	7.82	18
	N,N-dimethyl formamide	7.81	18
$C_3H_7NO_2$	nitropropane	8.5	2†
C_3H_8O	2-propanol	7.61	2
		6.97	18
	1-propanol	6.74	2
	ethyl methyl ether	7.93	2
$C_3H_8O_2$	dimethoxymethane	7.7	2†
	ethylene glycol monomethyl ether	7.44	27
C_3H_9N	propylamine	7.70	27
		9.20	2
	isopropylamine	7.77	27
	trimethylamine	8.15	2
		7.78*	33
$C_4H_2N_2$	fumaronitrile	11.8	2
$C_4H_4N_2$	succinonitrile	8.1	2†
	pyrimidine	8.53*	17
	pyridazine	9.27*	17
$C_4H_4O_2$	diketene	8.0	2†
C_4H_4S	thiophene	9.67	2
C_4H_5N	methacrylonitrile	8.0	2†
	trans-crotononitrile	8.2	2†
$C_4H_6N_2$	*N*-methylpyrazole	8.99	27
C_4H_6O	crotonaldehyde	8.5	2†
	methacrylaldehyde	8.3	2†
$C_4H_6O_2$	biacetyl	8.2	2†
$C_4H_6O_3$	acetic anhydride	8.9	2†
C_4H_6S	divinyl sulfide	10.9	2†
C_4H_7N	butyronitrile	8.4	2†
	isobutyronitrile	8.05	18
		8.05*	32
C_4H_8O	butanal	8.2	2†
	methyl ethyl ketone	8.13	15
	trans-2,3-epoxy butane	8.22*	17
$C_4H_8O_2$	ethyl acetate	9.7	2
		8.62	27

Molecule	Name	Polarizability	Ref.
	1,4-dioxane	10.0	2
	p-dioxane	8.60	18
	2-methyl-1,3-dioxolane	9.44	15
	butyric acid	8.58	27
	methyl propionate	8.97	27
$C_4H_9NO_2$	1-nitrobutane	10.4	2†
	2-methyl-2-nitropropane	10.3	2†
$C_4H_{10}O$	ethyl ether	10.2	2
		8.73	15
	1-butanol	8.88	2
	2-methylpropanol	8.92	2
	methyl propyl ether	8.86	27
	ethylene glycol monoethyl ether	9.28	27
$C_4H_{10}S$	ethyl sulfide	10.8	2
$C_4H_{11}N$	butylamine	13.5	2
	diethylamine	10.2	2
		9.61	27
C_5H_5N	pyridine	9.5	15
		9.18	27
	4-cyano-1,3-butadiene	10.5	2†
$C_5H_8N_2$	1,5-dimethylpyrazole	10.72	27
$C_5H_8O_2$	acetyl acetone	10.5	2†
C_5H_9N	valeronitrile	10.4	2
	22-DMPN	9.59	18
$C_5H_{10}O$	diethyl ketone	9.93	15
	methyl propyl ketone	9.93	15
$C_5H_{10}O_2$	ethyl propionate	10.41	27
	methyl butanoate	10.41	27
$C_5H_{10}O_3$	diethyl carbonate	11.3	2
$C_5H_{12}O$	ethyl propyl ether	10.68	27
$C_5H_{12}O_4$	tetramethyl orthocarbonate	13.0	2†
$C_6H_4N_2O_4$	*p*-dinitrobenzene	18.4	2
$C_6H_4O_2$	*p*-benzoquinone	14.5	2
$C_6H_5NO_2$	nitrobenzene	14.7	2
		12.92	15
C_6H_6O	phenol	11.1	2†
		9.94*	17
C_6H_7N	aniline	12.1	2†
$C_6H_8N_2$	phenylenediamine	13.8	2†
	phenylhydrazine	12.91	27
$C_6H_{10}N_2$	1-ethyl-5-methylpyrazole	12.50	27
$C_6H_{10}O_3$	ethyl acetoacetate	12.9	2†
$C_6H_{12}N_2$	dimethylketazine	15.6	2
$C_6H_{12}O$	cyclohexanol	11.56	18
$C_6H_{12}O_2$	amyl formate	14.2	2
$C_6H_{12}O_3$	paraldehyde	17.9	2
$C_6H_{14}O$	propyl ether	12.8	2
		12.5	15
$C_6H_{14}O_2$	1,1-diethoxyethane	13.2	2†
	1,2-diethoxyethane	11.3	2†
$C_6H_{15}N$	triethylamine	13.1	2
		13.38	27
	dipropylamine	13.29	27
$C_7H_4N_2O_2$	*p*-cyanonitrobenzene	19.0	2
C_7H_5N	benzonitrile	12.5	2†
$C_7H_7NO_3$	nitroanisole	15.7	2†
C_7H_8O	anisole	13.1	2†
C_7H_9NO	*o*-anisidine	14.2	2†
$C_7H_{10}N_2$	1,1-methylphenylhydrazine	14.81	27
$C_7H_{14}O$	cyclohexyl methyl ether	13.4	2†
	2,4-dimethyl-3-pentanone	13.5	15
$C_7H_{14}O_2$	pentyl acetate	14.9	2
$C_8H_4N_2$	*p*-dicyanobenzene	19.2	2

Molecule	Name	Polarizability	Ref.
$C_8H_6N_2$	quinoxaline	15.13	27
C_8H_8O	acetophenone	15.0	2
$C_8H_8O_2$	2,5-dimethyl-1,4-benzoquinone	18.8	2
$C_8H_{10}O$	phenetole	14.9	2
$C_8H_{11}N$	*N*-dimethylaniline	16.2	2†
$C_8H_{12}N_2$	1,1-ethylphenylhydrazine	16.62	27
$C_8H_{12}O_2$	ethyl sorbate	17.2	2†
	tetramethylcyclobutane-1,3-dione	18.6	2
$C_8H_{14}O_4$	diethyl succinate	16.8	2†
$C_8H_{18}O$	butyl ether	17.2	2
C_9H_7N	quinoline	15.70	27
	isoquinoline	16.43	27
$C_9H_{10}O_2$	ethyl benzoate	16.9	2†
$C_9H_{21}N$	tripropylamine	18.87	27
$C_{10}H_9N$	α-naphthylamine	19.50	27
	β-naphthylamine	19.73	27
	2-methylquinoline	18.65	27
	1-methylisoquinoline	18.28	27
$C_{10}H_{10}Fe$	ferrocene	17.1	26
$C_{10}H_{10}N_2$	2,3-dimethylquinoxaline	18.70	27
$C_{10}H_{14}BeO_4$	beryllium acetylacetonate	34.1	2
$C_{11}H_8O$	1-naphthaldehyde	19.75	27
	2-naphthaldehyde	20.06	27
$C_{12}H_8N_2$	phenazine	23.43	27
$C_{12}H_9NO_3$	4-nitrodiphenyl ether	24.7	2†
$C_{14}H_8O_2$	anthraquinone	24.46	27
$C_{14}H_{14}O$	di-*p*-tolyl ether	24.9	2†
$C_{15}H_{21}AlO_6$	aluminum acetylacetonate	51.9	2
$C_{15}H_{21}CrO_6$	chromium acetylacetonate	53.7	2
$C_{15}H_{21}FeO_6$	ferric acetylacetonate	58.1	2
$C_{20}H_{28}O_8Th$	thorium acetylacetonate	79.0	2
C_{60}	buckminsterfullerene	76.5	24
		79	31

Note: All polarizabilities in the tables are experimental values except those values marked by an asterisk (*), which indicates a calculated result. The experimental polarizabilities are mostly determined by measurements of a dielectric constant or refractive index which are quite accurate (0.5% or better). However, one should treat many of the results with several percent of caution because of the age of the data and because some of the results refer to optical frequencies rather than static. Comments given with the references are intended to allow one to judge the degree of caution required. Interested persons should consult these references. In many cases, the reference given is to a theoretical paper in which the experimental results are quoted. These papers, noted in the References, contain valuable information on polarizability calculations and experimental data which often includes the tensor components of the polarizability.

An emperical additive formula for molecular polarizabilities at 589 nm frequency has been given in Bosque, R., and Sales, J., *J. Chem. Inf. Comput. Sci.* 42, 1154, 2002: α=0.32 +1.51#C +0.17#H +0.57#O +1.05#N +2.99#S +2.48#P +2.16#Cl +3.29#Br +5.45#I, where "#C" denotes the number of carbon atoms in the molecule, etc.

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