Dipolmomente einiger Moleküle

TABLE 4.1 Dipole moments of molecules, bonds, and molecular groups (in Debye units: $1\,D = 3.336 \times 10^{-30}\,C\,m)^a$

Molecules

Alkanes	0^b	H_2O	1.85
C_6H_6 (benzene)	0	CH_3OH, C_2H_5OH	1.7
CCl_4	0	Hexanol, octanol	1.7
CO_2	0	$C_6H_{11}OH$ (cyclohexanol)	1.7
CO	0.11	CH_3COOH (acetic acid)	1.7
$CHCl_3$ (chloroform)	1.06	C_2H_4O (ethylene oxide)	1.9
HCl	1.08	CH_3COCH_3 (acetone)	2.9
NH_3	1.47	$HCONH_2$ (formamide)	3.7
SO_2	1.62	C_6H_5OH (phenol)	1.5
CH_3Cl	1.87	$C_6H_5NH_2$ (aniline)	1.5
NaCl	8.5	C_6H_5Cl (chlorobenzene)	1.8
CsCl	10.4	$C_6H_5NO_2$ (nitrobenzene)	4.2

Bond moments

$C—H^+$	0.4	$C—C$	0	$C^+—Cl$	1.5–1.7
$N—H^+$	1.31	$C=C$	0	$N^+—O$	0.3
$O—H^+$	1.51	$C^+—N$	0.22	$C^+=O$	2.3–2.7
$F—H^+$	1.94	$C^+—O$	0.74	$N^+=O$	2.0

Group moments

$C—^+OH$	1.65	$C—^+CH_3$	0.4	$C—^+COOH$	1.7
$C—^+NH_2$	1.2–1.5	$C^+—NO_2$	3.1–3.8	$C—^+OCH_3$	1.3

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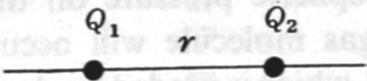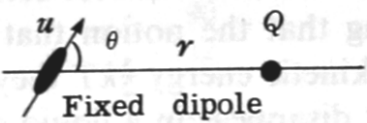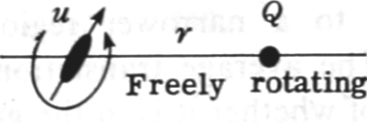
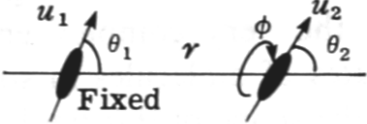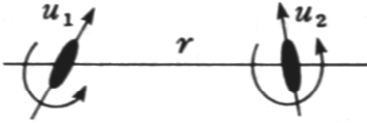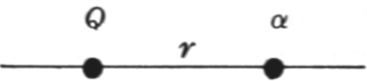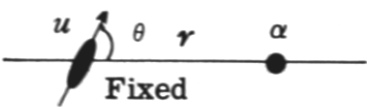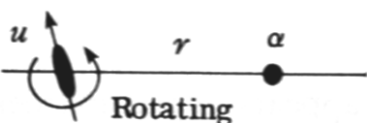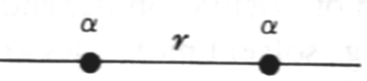# Polarisierbarkeit einiger Moleküle

TABLE 5.1 Electronic polarizabilities α_0 of atoms, molecules, bonds, and molecular groups[a]

Atoms and molecules

He	0.20	NH_3	2.3	$CH_2{=}CH_2$	4.3
H_2	0.81	CH_4	2.6	C_2H_6	4.5
H_2O	1.48	HCl	2.6	Cl_2	4.6
O_2	1.60	CO_2	2.6	$CHCl_3$	8.2
Ar	1.63	CH_3OH	3.2	C_6H_6	10.3
CO	1.95	Xe	4.0	CCl_4	10.5

Bond polarizabilities

Aliphatic	C—C	0.48		C—O	0.60
Aromatic	C⋯C	1.07		C=O	1.36
	C=C	1.65		N—H	0.74
Aliphatic	C—H	0.65		C—Cl	2.60
	O—H	0.73		C—Br	3.75

Molecular groups

C—O—H	1.28	CH_2		1.84
C—O—C	1.13	Si—O—Si		1.39
C—NH_2	2.03	Si—OH		1.60

[a] Polarizabilities α_0 are given in units of $(4\pi\varepsilon_0)Å^3 = (4\pi\varepsilon_0)10^{-30}\,m^3 = 1.11 \times 10^{-40}\,C^2\,m^2\,J^{-1}$. Note that when molecules are dissolved in a solvent medium their polarizability can change by up to 10%. Data compiled from Denbigh (1940), Hirschfelder *et al.* (1954) and Smyth (1955).
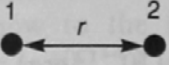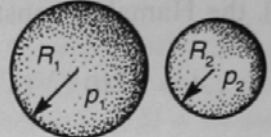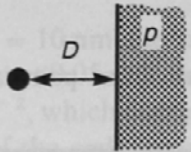
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Übersicht Wechselwirkungen
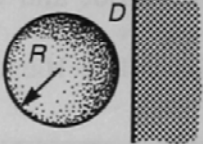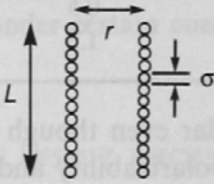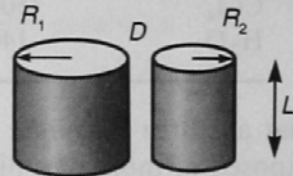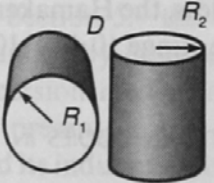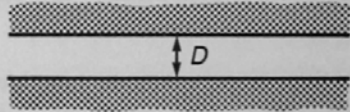
Charge–charge	Q_1 $\quad r \quad$ Q_2	$Q_1 Q_2/4\pi\varepsilon_0 r$ (Coulomb energy)
	$u\ \theta \quad r \quad Q$ Fixed dipole	$-Qu\cos\theta/4\pi\varepsilon_0 r^2$
Charge–dipole	$u \quad r \quad Q$ Freely rotating	$-Q^2 u^2/6(4\pi\varepsilon_0)^2 kTr^4$
	$u_1\ \theta_1 \quad r \quad \phi\ \theta_2\ u_2$ Fixed	$-u_1 u_2[2\cos\theta_1\cos\theta_2 - \sin\theta_1\sin\theta_2\cos\phi]/4\pi\varepsilon_0 r^3$
Dipole–dipole	$u_1 \quad r \quad u_2$ Freely rotating	$-u_1^2 u_2^2/3(4\pi\varepsilon_0)^2 kTr^6$ (Keesom energy)
Charge–non-polar	$Q \quad r \quad \alpha$	$-Q^2\alpha/2(4\pi\varepsilon_0)^2 r^4$
	$u\ \theta \quad r \quad \alpha$ Fixed	$-u^2\alpha(1 + 3\cos^2\theta)/2(4\pi\varepsilon_0)^2 r^6$
Dipole–non-dipolar	$u \quad r \quad \alpha$ Rotating	$-u^2\alpha/(4\pi\varepsilon_0)^2 r^6$ (Debye energy)
Two non-polar molecules	$\alpha \quad r \quad \alpha$	$\dfrac{3}{4}\dfrac{h\nu\alpha^2}{(4\pi\varepsilon_0)^2 r^6}$ (London dispersion energy)

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Relative Stärke der verschiedenen Van der Waals - Wechselwirkungen

Interacting molecules	Electronic polarizability $\dfrac{\alpha_0}{4\pi\varepsilon_0}$ $(10^{-30}\,m^3)$	Permanent dipole moment u $(D)^a$	Ionization potential $I = h\nu_I$ $(eV)^b$	Induktion (Debye) $\dfrac{C_{ind}}{\dfrac{2u^2\alpha_0}{(4\pi\varepsilon_0)^2}}$	Orientierung (Keesom) $\dfrac{C_{orient}}{\dfrac{u^4/3kT}{(4\pi\varepsilon_0)^2}}$	Dispersion (London) $\dfrac{C_{disp}}{\dfrac{3\alpha_0^2 h\nu_I}{4(4\pi\varepsilon_0)^2}}$
Ne–Ne	0.39	0	21.6	0	4	4
CH_4–CH_4	2.60	0	12.6	0	0	102
HCl–HCl	2.63	1.08	12.7	6	11	106
HBr–HBr	3.61	0.78	11.6	4	3	182
HI–HI	5.44	0.38	10.4	2	0.2	370
CH_3Cl–CH_3Cl	4.56	1.87	11.3	32	101	282
NH_3–NH_3	2.26	1.47	10.2	10	38	63
H_2O–H_2O	1.48	1.85	12.6	10	96	33
Dissimilar molecules				$\dfrac{u_1^2\alpha_{02} + u_2^2\alpha_{01}}{(4\pi\varepsilon_0)^2}$	$\dfrac{u_1^2 u_2^2/3kT}{(4\pi\varepsilon_0)^2}$	$\dfrac{3\alpha_{01}\alpha_{02}h\nu_1\nu_2}{2(4\pi\varepsilon_0)^2(\nu_1+\nu_2)}$
Ne–CH_4				0	0	19
HCl–HI				7	1	197
H_2O–Ne				1	0	11
H_2O–CH_4				9	0	58

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Two atoms

$w = -C/r^6$

Two spheres

$W = \dfrac{-A}{6D} \dfrac{R_1 R_2}{(R_1 + R_2)}$

Atom–surface

$w = -\pi C p / 6D^3$

Sphere–surface

$W = -AR/6D$

Two parallel chain molecules

$W = -3\pi C L / 8\sigma^2 r^5$

Two cylinders

$W = \dfrac{AL}{12\sqrt{2}\,D^{3/2}} \left(\dfrac{R_1 R_2}{R_1 + R_2} \right)^{1/2}$

Two crossed cylinders

$W = -A\sqrt{R_1 R_2}/6D$

Two surfaces

$W = -A/12\pi D^2$ per unit area

Wechselwirkungen zwischen verschiedenen ausgedehnten Objekten

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