Data section

The following tables reproduce and expand the data given in the short tables in the text, and follow their numbering. Standard states refer to a pressure of $p^{\ominus} = 1$ bar. The general references are as follows:

AIP: D.E. Gray (ed.), *American Institute of Physics handbook.* McGraw-Hill, New York (1972).

AS: M. Abramowitz and I.A. Stegun (ed.), *Handbook of mathematical functions.* Dover, New York (1963).

E: J. Emsley, *The elements.* Oxford University Press (1991).

HCP: R.C. Weast (ed.), *Handbook of chemistry and physics.* CRC Press, Boca Raton (1993).

JL: A.M. James and M.P. Lord, *Macmillan's chemical and physical data.* Macmillan, London (1992).

KL: G.W.C. Kaye and T.H. Laby (ed.), *Tables of physical and chemical constants.* Longman, London (1973).

LR: G.N. Lewis and M. Randall, revised by K.S. Pitzer and L. Brewer, *Thermodynamics.* McGraw-Hill, New York (1961).

NBS: *NBS tables of chemical thermodynamic properties*, published as *J. Phys. and Chem. Reference Data*, **11**, Supplement 2 (1982).

RS: R.A. Robinson and R.H. Stokes, *Electrolyte solutions.* Butterworth, London (1959).

TDOC: J.B. Pedley, J.D. Naylor, and S.P. Kirby, *Thermochemical data of organic compounds.* Chapman & Hall, London (1986).

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Physical properties of selected materials

	ρ/(g cm^{-3}) at 293 K†	T_f/K	T_b/K		ρ/(g cm^{-3}) at 293 K†	T_f/K	T_b/K
Elements				Inorganic compounds			
Aluminium(s)	2.698	933.5	2740	$CaCO_3$(s, calcite)	2.71	1612	1171d
Argon(g)	1.381	83.8	87.3	$CuSO_4{\cdot}5H_2O$(s)	2.284	383(−H_2O)	423(−$5H_2O$)
Boron(s)	2.340	2573	3931	HBr(g)	2.77	184.3	206.4
Bromine(l)	3.123	265.9	331.9	HCl(g)	1.187	159.0	191.1
Carbon(s, gr)	2.260	3700s		HI(g)	2.85	222.4	237.8
Carbon(s, d)	3.513			H_2O(l)	0.997	273.2	373.2
Chlorine(g)	1.507	172.2	239.2	D_2O(l)	1.104	277.0	374.6
Copper(s)	8.960	1357	2840	NH_3(g)	0.817	195.4	238.8
Fluorine(g)	1.108	53.5	85.0	KBr(s)	2.750	1003	1708
Gold(s)	19.320	1338	3080	KCl(s)	1.984	1049	1773s
Helium(g)	0.125		4.22	NaCl(s)	2.165	1074	1686
Hydrogen(g)	0.071	14.0	20.3	H_2SO_4(l)	1.841	283.5	611.2
Iodine(s)	4.930	386.7	457.5	Organic compounds			
Iron(s)	7.874	1808	3023	Acetaldehyde, CH_3CHO(l, g)	0.788	152	293
Krypton(g)	2.413	116.6	120.8	Acetic acid, CH_3COOH(l)	1.049	289.8	391
Lead(s)	11.350	600.6	2013	Acetone, $(CH_3)_2CO$(l)	0.787	178	329
Lithium(s)	0.534	453.7	1620	Aniline, $C_6H_5NH_2$(l)	1.026	267	457
Magnesium(s)	1.738	922.0	1363	Anthracene, $C_{14}H_{10}$(s)	1.243	490	615
Mercury(l)	13.546	234.3	629.7	Benzene, C_6H_6(l)	0.879	278.6	353.2
Neon(g)	1.207	24.5	27.1	Carbon tetrachloride, CCl_4(l)	1.63	250	349.9
Nitrogen(g)	0.880	63.3	77.4	Chloroform, $CHCl_3$(l)	1.499	209.6	334
Oxygen(g)	1.140	54.8	90.2	Ethanol, C_2H_5OH(l)	0.789	156	351.4
Phosphorus(s, wh)	1.820	317.3	553	Formaldehyde, HCHO(g)		181	254.0
Potassium(s)	0.862	336.8	1047	Glucose, $C_6H_{12}O_6$(s)	1.544	415	
Silver(s)	10.500	1235	2485	Methane, CH_4(g)		90.6	111.6
Sodium(s)	0.971	371.0	1156	Methanol, CH_3OH(l)	0.791	179.2	337.6
Sulfur(s, α)	2.070	386.0	717.8	Naphthalene, $C_{10}H_8$(s)	1.145	353.4	491
Uranium(s)	18.950	1406	4018	Octane, C_8H_{18}(l)	0.703	216.4	398.8
Xenon(g)	2.939	161.3	166.1	Phenol, C_6H_5OH(s)	1.073	314.1	455.0
Zinc(s)	7.133	692.7	1180	Sucrose, $C_{12}H_{22}O_{11}$(s)	1.588	457d	

d: decomposes; s: sublimes; Data: AIP, E, HCP, KL; † For gases, at their boiling points.

Table 1.3 Collision cross-sections, σ/nm^2

Ar	0.36
C_2H_4	0.64
C_6H_6	0.88
CH_4	0.46
Cl_2	0.93
CO_2	0.52
H_2	0.27
He	0.21
N_2	0.43
Ne	0.24
O_2	0.40
SO_2	0.58

Data: KL

Table 1.4 Second virial coefficients, $B/(cm^3\ mol^{-1})$

	100 K	273 K	373 K	600 K
Air	−167.3	−13.5	3.4	19.0
Ar	−187.0	−21.7	−4.2	11.9
CH_4		−53.6	−21.2	8.1
CO_2		−142	−72.2	−12.4
H_2	−2.0	13.7	15.6	
He	11.4	12.0	11.3	10.4
Kr		−62.9	−28.7	1.7
N_2	−160.0	−10.5	6.2	21.7
Ne	−6.0	10.4	12.3	13.8
O_2	−197.5	−22.0	−3.7	12.9
Xe		−153.7	−81.7	−19.6

Data: AIP, JL. The values relate to the expansion in eqn 36 of Section 1.4b; convert to eqn 35 using $B' = B/RT$.
For Ar at 273 K, $C = 1200\ cm^6\ mol^{-1}$

Table 1.5 Critical constants

	p_c/atm	$V_c/(cm^3\ mol^{-1})$	T_c/K	Z_c	T_B/K		p_c/atm	$V_c/(cm^3\ mol^{-1})$	T_c/K	Z_c	T_B/K
Ar	48.00	75.25	150.72	0.292	411.5	HCl	81.5	81.0	324.7	0.248	
Br_2	102	135	584	0.287		He	2.26	57.76	5.21	0.305	22.64
C_2H_4	50.50	124	283.1	0.270		HI	80.8	423.2			
C_2H_6	48.20	148	305.4	0.285		Kr	54.27	92.24	209.39	0.291	575.0
C_6H_6	48.6	260	562.7	0.274		N_2	33.54	90.10	126.3	0.292	327.2
CH_4	45.6	98.7	190.6	0.288	510.0	Ne	26.86	41.74	44.44	0.307	122.1
Cl_2	76.1	124	417.2	0.276		NH_3	111.3	72.5	405.5	0.242	
CO_2	72.85	94.0	304.2	0.274	714.8	O_2	50.14	78.0	154.8	0.308	405.9
F_2	55	144				Xe	58.0	118.8	289.75	0.290	768.0
H_2	12.8	64.99	33.23	0.305	110.0						
H_2O	218.3	55.3	647.4	0.227							
HBr	84.0	363.0									

Data: AIP, KL

Table 1.6 van der Waals constants

	$a/(atm\ L^2\ mol^{-2})$	$b/(10^{-2}\ L\ mol^{-1})$		$a/(atm\ L^2\ mol^{-2})$	$b/(10^{-2}\ L\ mol^{-1})$
Ar	1.363	3.219	H_2S	4.490	4.287
C_2H_4	4.530	5.714	He	0.03457	2.370
C_2H_6	5.562	6.380	Kr	2.349	3.978
C_6H_6	18.24	11.54	N_2	1.408	3.913
CH_4	2.283	4.278	Ne	0.2135	1.709
Cl_2	6.579	5.622	NH_3	4.225	3.707
CO	1.505	3.985	O_2	1.378	3.183
CO_2	3.640	4.267	SO_2	6.803	5.636
H_2	0.2476	2.661	Xe	4.250	5.105
H_2O	5.536	3.049			

Data: HCP, JL

Table 2.2 Temperature variation of molar heat capacities†

	a	$b/(10^{-3}\,\mathrm{K})$	$c/(10^{5}\,\mathrm{K})$
Monatomic gases			
	20.78	0	0
Other gases			
Br_2	37.32	0.50	−1.26
Cl_2	37.03	0.67	−2.85
CO_2	44.22	8.79	−8.62
F_2	34.56	2.51	−3.51
H_2	27.28	3.26	0.50
I_2	37.40	0.59	−0.71
N_2	28.58	3.77	−0.50
NH_3	29.75	25.1	−1.55
O_2	29.96	4.18	−1.67
Liquids (from melting to boiling)			
$C_{10}H_8$, naphthalene	79.5	0.4075	0
I_2	80.33	0	0
H_2O	75.29	0	0
Solids			
Al	20.67	12.38	0
C (graphite)	16.86	4.77	−8.54
$C_{10}H_8$, naphthalene	−115.9	3.920×10^{3}	0
Cu	22.64	6.28	0
I_2	40.12	49.79	0
NcCl	45.94	16.32	0
Pb	22.13	11.72	0.96

† For $C_{p,m}/(\mathrm{J\,K^{-1}\,mol^{-1}}) = a + bT + c/T^2$
Source: LR.

Table 2.3 Standard enthalpies of fusion and vaporization at the transition temperature, $\Delta_{trs}H^{\ominus}/(\mathrm{kJ\,mol^{-1}})$

	T_f/K	Fusion	T_b/K	Vaporization
Elements				
Ag	1234	11.30	2436	250.6
Ar	83.81	1.188	87.29	6.506
Br_2	265.9	10.57	332.4	29.45
Cl_2	172.1	6.41	239.1	20.41
F_2	53.6	0.26	85.0	3.16
H_2	13.96	0.117	20.38	0.916
He	3.5	0.021	4.22	0.084
Hg	234.3	2.292	629.7	59.30
I_2	386.8	15.52	458.4	41.80
N_2	63.15	0.719	77.35	5.586
Na	371.0	2.601	1156	98.01
O_2	54.36	0.444	90.18	6.820
Xe	161	2.30	165	12.6
K	336.4	2.35	1031	80.23
Inorganic compounds				
CCl_4	250.3	2.47	349.9	30.00
CO_2	217.0	8.33	194.6	25.23 s
CS_2	161.2	4.39	319.4	26.74
H_2O	273.15	6.008	373.15	40.656
				44.016 at 298 K
H_2S	187.6	2.377	212.8	18.67
H_2SO_4	283.5	2.56		
NH_3	195.4	5.652	239.7	23.35
Organic compounds				
CH_4	90.68	0.941	111.7	8.18
CCl_4	250.3	2.5	350	30.0
C_2H_6	89.85	2.86	184.6	14.7
C_6H_6	278.61	10.59	353.2	30.8
C_6H_{14}	178	13.08	342.1	28.85
$C_{10}H_8$	354	18.80	490.9	51.51
CH_3OH	175.2	3.16	337.2	35.27
				37.99 at 298 K
C_2H_5OH	158.7	4.60	352	43.5

Data: AIP; s denotes sublimation

Table 2.5 Thermodynamic data for organic compounds (all values are for 298 K)

	M/(g mol^{-1})	$\Delta_f H^\ominus$/(kJ mol^{-1})	$\Delta_f G^\ominus$/(kJ mol^{-1})	$S^\ominus_m$/(J K^{-1} mol^{-1})	$C^\ominus_{p,m}$/(J K^{-1} mol^{-1})	$\Delta_c H^\ominus$/(kJ mol^{-1})
C(s) (graphite)	12.011	0	0	5.740	8.527	−393.51
C(s) (diamond)	12.011	+1.895	+2.900	2.377	6.113	−395.40
CO_2(g)	44.010	−393.51	−394.36	213.74	37.11	
Hydrocarbons						
CH_4(g), methane	16.04	−74.81	−50.72	186.26	35.31	−890
CH_3(g), methyl	15.04	+145.69	+147.92	194.2	38.70	
C_2H_2(g), ethyne	26.04	+226.73	+209.20	200.94	43.93	−1300
C_2H_4(g), ethene	28.05	+52.26	+68.15	219.56	43.56	−1411
C_2H_6(g), ethane	30.07	−84.68	−32.82	229.60	52.63	−1560
C_3H_6(g), propene	42.08	+20.42	+62.78	267.05	63.89	−2058
C_3H_6(g), cyclopropane	42.08	+53.30	+104.45	237.55	55.94	−2091
C_3H_8(g), propane	44.10	−103.85	−23.49	269.91	73.5	−2220
C_4H_8(g), 1-butene	56.11	−0.13	+71.39	305.71	85.65	−2717
C_4H_8(g), *cis*-2-butene	56.11	−6.99	+65.95	300.94	78.91	−2710
C_4H_8(g), *trans*-2-butene	56.11	−11.17	+63.06	296.59	87.82	−2707
C_4H_{10}(g), butane	58.13	−126.15	−17.03	310.23	97.45	−2878
C_5H_{12}(g), pentane	72.15	−146.44	−8.20	348.40	120.2	−3537
C_5H_{12}(l)	72.15	−173.1				
C_6H_6(l), benzene	78.12	+49.0	+124.3	173.3	136.1	−3268
C_6H_6(g)	78.12	+82.93	+129.72	269.31	81.67	−3302
C_6H_{12}(l), cyclohexane	84.16	−156	+26.8		156.5	−3920
C_6H_{14}(l), hexane	86.18	−198.7		204.3		−4163
$C_6H_5CH_3$(g), methyl-benzene (toluene)	92.14	+50.0	+122.0	320.7	103.6	−3953
C_7H_{16}(l), heptane	100.21	−224.4	+1.0	328.6	224.3	
C_8H_{18}(l), octane	114.23	−249.9	+6.4	361.1		−5471
C_8H_{18}(l), iso-octane	114.23	−255.1				−5461
$C_{10}H_8$(s), naphthalene	128.18	+78.53				−5157
Alcohols and phenols						
CH_3OH(l), methanol	32.04	−238.66	−166.27	126.8	81.6	−726
CH_3OH(g)	32.04	−200.66	−161.96	239.81	43.89	−764
C_2H_5OH(l), ethanol	46.07	−277.69	−174.78	160.7	111.46	−1368
C_2H_5OH(g)	46.07	−235.10	−168.49	282.70	65.44	−1409
C_6H_5OH(s), phenol	94.12	−165.0	−50.9	146.0		−3054
Carboxylic acids, hydroxy acids, and esters						
HCOOH(l), formic	46.03	−424.72	−361.35	128.95	99.04	−255
CH_3COOH(l), acetic	60.05	−484.5	−389.9	159.8	124.3	−875
CH_3COOH(aq)	60.05	−485.76	−396.46	178.7		
$CH_3CO_2^-$(aq)	59.05	−486.01	−369.31	86.6	−6.3	
$(COOH)_2$(s), oxalic	90.04	−827.2			117	−254
C_6H_5COOH(s), benzoic	122.13	−385.1	−245.3	167.6	146.8	−3227
$CH_3CH(OH)COOH$(s), lactic	90.08	−694.0				−1344
$CH_3COOC_2H_5$(l), ethyl acetate	88.11	−479.0	−332.7	259.4	170.1	−2231
Alkanals and alkanones						
HCHO(g), methanal	30.03	−108.57	−102.53	218.77	35.40	−571
CH_3CHO(l), ethanal	44.05	−192.30	−128.12	160.2		−1166
CH_3CHO(g)	44.05	−166.19	−128.86	250.3	57.3	−1192
CH_3COCH_3(l), propanone	58.08	−248.1	−155.4	200.4	124.7	−1790

Table 2.5 (Continued)

	M/(g mol^{-1})	$\Delta_f H^\ominus$/(kJ mol^{-1})	$\Delta_f G^\ominus$/(kJ mol^{-1})	$S^\ominus_m$/(J K^{-1} mol^{-1})	$C^\ominus_{p,m}$/(J K^{-1} mol^{-1})	$\Delta_c H^\ominus$/(kJ mol^{-1})
Sugars						
$C_6H_{12}O_6$(s), α-D-glucose	180.16	−1274				−2808
$C_6H_{12}O_6$(s), β-D-glucose	180.16	−1268	−910	212		
$C_6H_{12}O_6$(s), β-D-fructose	180.16	−1266				−2810
$C_{12}H_{22}O_{11}$(s), sucrose	342.30	−2222	−1543	360.2		−5645
Nitrogen compounds						
$CO(NH_2)_2$(s), urea	60.06	−333.51	−197.33	104.60	93.14	−632
CH_3NH_2(g), methylamine	31.06	−22.97	+32.16	243.41	53.1	−1085
$C_6H_5NH_2$(l), aniline	93.13	+31.1				−3393
$CH_2(NH_2)COOH$(s), glycine	75.07	−532.9	−373.4	103.5	99.2	−969

Data: NBS, TDOC

Table 2.6 Thermodynamic data (all values relate to 298 K)

	M/(g mol^{-1})	$\Delta_f H^\ominus$/(kJ mol^{-1})	$\Delta_f G^\ominus$/(kJ mol^{-1})	$S^\ominus_m$/(J K^{-1} mol^{-1})	$C^\ominus_{p,m}$/(J K^{-1} mol^{-1})
Aluminium (aluminum)					
Al(s)	26.98	0	0	28.33	24.35
Al(l)	26.98	+10.56	+7.20	39.55	24.21
Al(g)	26.98	+326.4	+285.7	164.54	21.38
Al^{3+}(g)	26.98	+5483.17			
Al^{3+}(aq)	26.98	−531	−485	−321.7	
Al_2O_3(s, α)	101.96	−1675.7	−1582.3	50.92	79.04
$AlCl_3$(s)	133.24	−704.2	−628.8	110.67	91.84
Argon					
Ar(g)	39.95	0	0	154.84	20.786
Antimony					
Sb(s)	121.75	0	0	45.69	25.23
SbH_3(g)	124.77	+145.11	+147.75	232.78	41.05
Arsenic					
As(s, α)	74.92	0	0	35.1	24.64
As(g)	74.92	+302.5	+261.0	174.21	20.79
As_4(g)	299.69	+143.9	+92.4	314	
AsH_3(g)	77.95	+66.44	+68.93	222.78	38.07
Barium					
Ba(s)	137.34	0	0	62.8	28.07
Ba(g)	137.34	+180	+146	170.24	20.79
Ba^{2+}(aq)	137.34	−537.64	−560.77	9.6	
BaO(s)	153.34	−553.5	−525.1	70.43	47.78
$BaCl_2$(s)	208.25	−858.6	−810.4	123.68	75.14
Beryllium					
Be(s)	9.01	0	0	9.50	16.44
Be(g)	9.01	+324.3	+286.6	136.27	20.79

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Table 2.6 (Continued)

	M/(g mol^{-1})	$\Delta_f H^\ominus$/(kJ mol^{-1})	$\Delta_f G^\ominus$/(kJ mol^{-1})	$S^\ominus_m$/(J K^{-1} mol^{-1})	$C^\ominus_{p,m}$/(J K^{-1} mol^{-1})
Hydrogen (Continued)					
$H_2O(l)$	18.015	−285.83	−237.13	69.91	75.291
$H_2O(g)$	18.015	−241.82	−228.57	188.83	33.58
$H_2O_2(l)$	34.015	−187.78	−120.35	109.6	89.1
Iodine					
$I_2(s)$	253.81	0	0	116.135	54.44
$I_2(g)$	253.81	+62.44	+19.33	260.69	36.90
$I(g)$	126.90	+106.84	+70.25	180.79	20.786
$I^-(aq)$	126.90	−55.19	−51.57	111.3	−142.3
$HI(g)$	127.91	+26.48	+1.70	206.59	29.158
Iron					
$Fe(s)$	55.85	0	0	27.28	25.10
$Fe(g)$	55.85	+416.3	+370.7	180.49	25.68
$Fe^{2+}(aq)$	55.85	−89.1	−78.90	−137.7	
$Fe^{3+}(aq)$	55.85	−48.5	−4.7	−315.9	
$Fe_3O_4(s)$ (magnetite)	231.54	−1118.4	−1015.4	146.4	143.43
$Fe_2O_3(s)$ (haematite)	159.69	−824.2	−742.2	87.40	103.85
$FeS(s, \alpha)$	87.91	−100.0	−100.4	60.29	50.54
$FeS_2(s)$	119.98	−178.2	−166.9	52.93	62.17
Krypton					
$Kr(g)$	83.80	0	0	164.08	20.786
Lead					
$Pb(s)$	207.19	0	0	64.81	26.44
$Pb(g)$	207.19	+195.0	+161.9	175.37	20.79
$Pb^{2+}(aq)$	207.19	−1.7	−24.43	10.5	
PbO(s, yellow)	223.19	−217.32	−187.89	68.70	45.77
PbO(s, red)	223.19	−218.99	−188.93	66.5	45.81
$PbO_2(s)$	239.19	−277.4	−217.33	68.6	64.64
Lithium					
$Li(s)$	6.94	0	0	29.12	24.77
$Li(g)$	6.94	+159.37	+126.66	138.77	20.79
$Li^+(aq)$	6.94	−278.49	−293.31	13.4	68.6
Magnesium					
$Mg(s)$	24.31	0	0	32.68	24.89
$Mg(g)$	24.31	+147.70	+113.10	148.65	20.786
$Mg^{2+}(aq)$	24.31	−466.85	−454.8	−138.1	
$MgO(s)$	40.31	−601.70	−569.43	26.94	37.15
$MgCO_3(s)$	84.32	−1095.8	−1012.1	65.7	75.52
$MgCl_2(s)$	95.22	−641.32	−591.79	89.62	71.38
Mercury					
$Hg(l)$	200.59	0	0	76.02	27.983
$Hg(g)$	200.59	+61.32	+31.82	174.96	20.786
$Hg^{2+}(aq)$	200.59	+171.1	+164.40	−32.2	
$Hg_2^{2+}(aq)$	401.18	+172.4	+153.52	84.5	
$HgO(s)$	216.59	−90.83	−58.54	70.29	44.06

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Table 2.6 (Continued)

	$M/(\mathrm{g\,mol^{-1}})$	$\Delta_f H^\ominus/(\mathrm{kJ\,mol^{-1}})$	$\Delta_f G^\ominus/(\mathrm{kJ\,mol^{-1}})$	$S^\ominus_m/(\mathrm{J\,K^{-1}\,mol^{-1}})$	$C^\ominus_{p,m}/(\mathrm{J\,K^{-1}\,mol^{-1}})$
Mercury (Continued)					
$Hg_2Cl_2(s)$	472.09	−265.22	−210.75	192.5	102
$HgCl_2(s)$	271.50	−224.3	−178.6	146.0	
HgS(s, black)	232.65	−53.6	−47.7	88.3	
Neon					
Ne(g)	20.18	0	0	146.33	20.786
Nitrogen					
$N_2(g)$	28.013	0	0	191.61	29.125
N(g)	14.007	+472.70	+455.56	153.30	20.786
NO(g)	30.01	+90.25	+86.55	210.76	29.844
$N_2O(g)$	44.01	+82.05	+104.20	219.85	38.45
$NO_2(g)$	46.01	+33.18	+51.31	240.06	37.20
$N_2O_4(g)$	92.01	+9.16	+97.89	304.29	77.28
$N_2O_5(s)$	108.01	−43.1	+113.9	178.2	143.1
$N_2O_5(g)$	108.01	+11.3	+115.1	355.7	84.5
$HNO_3(l)$	63.01	−174.10	−80.71	155.60	109.87
$HNO_3(aq)$	63.01	−207.36	−111.25	146.4	−86.6
$NO_3^-(aq)$	62.01	−205.0	−108.74	146.4	−86.6
$NH_3(g)$	17.03	−46.11	−16.45	192.45	35.06
$NH_3(aq)$	17.03	−80.29	−26.50	111.3	
$NH_4^+(aq)$	18.04	−132.51	−79.31	113.4	79.9
$NH_2OH(s)$	33.03	−114.2			
$HN_3(l)$	43.03	+264.0	+327.3	140.6	43.68
$HN_3(g)$	43.03	+294.1	+328.1	238.97	98.87
$N_2H_4(l)$	32.05	+50.63	+149.43	121.21	139.3
$NH_4NO_3(s)$	80.04	−365.56	−183.87	151.08	84.1
$NH_4Cl(s)$	53.49	−314.43	−202.87	94.6	
Oxygen					
$O_2(g)$	31.999	0	0	205.138	29.355
O(g)	15.999	+249.17	+231.73	161.06	21.912
$O_3(g)$	47.998	+142.7	+163.2	238.93	39.20
$OH^-(aq)$	17.007	−229.99	−157.24	−10.75	−148.5
Phosphorus					
P(s, wh)	30.97	0	0	41.09	23.840
P(g)	30.97	+314.64	+278.25	163.19	20.786
$P_2(g)$	61.95	+144.3	+103.7	218.13	32.05
$P_4(g)$	123.90	+58.91	+24.44	279.98	67.15
$PH_3(g)$	34.00	+5.4	+13.4	210.23	37.11
$PCl_3(g)$	137.33	−287.0	−267.8	311.78	71.84
$PCl_3(l)$	137.33	−319.7	−272.3	217.1	
$PCl_5(g)$	208.24	−374.9	−305.0	364.6	112.8
$PCl_5(s)$	208.24	−443.5			
$H_3PO_3(s)$	82.00	−964.4			
$H_3PO_3(aq)$	82.00	−964.8			
$H_3PO_4(s)$	94.97	−1279.0	−1119.1	110.50	106.06
$H_3PO_4(l)$	94.97	−1266.9			
$H_3PO_4(aq)$	94.97	−1277.4	−1018.7	−222	

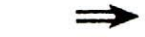

Table 2.6 (Continued)

	$M/(\mathrm{g\,mol^{-1}})$	$\Delta_f H^\ominus/(\mathrm{kJ\,mol^{-1}})$	$\Delta_f G^\ominus/(\mathrm{kJ\,mol^{-1}})$	$S_m^\ominus/(\mathrm{J\,K^{-1}\,mol^{-1}})$	$C_{p,m}^\ominus/(\mathrm{J\,K^{-1}\,mol^{-1}})$
Phosphorus (Continued)					
PO_4^{3-}(aq)	94.97	−1277.4	−1018.7	−221.8	
P_4O_{10}(s)	283.89	−2984.0	−2697.0	228.86	211.71
P_4O_6(s)	219.89	−1640.1			
Potassium					
K(s)	39.10	0	0	64.18	29.58
K(g)	39.10	+89.24	+60.59	160.336	20.786
K^+(g)	39.10	+514.26			
K^+(aq)	39.10	−252.38	−283.27	102.5	21.8
KOH(s)	56.11	−424.76	−379.08	78.9	64.9
KF(s)	58.10	−576.27	−537.75	66.57	49.04
KCl(s)	74.56	−436.75	−409.14	82.59	51.30
KBr(s)	119.01	−393.80	−380.66	95.90	52.30
KI(s)	166.01	−327.90	−324.89	106.32	52.93
Silicon					
Si(s)	28.09	0	0	18.83	20.00
Si(g)	28.09	+455.6	+411.3	167.97	22.25
SiO_2(s, α)	60.09	−910.94	−856.64	41.84	44.43
Silver					
Ag(s)	107.87	0	0	42.55	25.351
Ag(g)	107.87	+284.55	+245.65	173.00	20.79
Ag^+(aq)	107.87	+105.58	+77.11	72.68	21.8
AgBr(s)	187.78	−100.37	−96.90	107.1	52.38
AgCl(s)	143.32	−127.07	−109.79	96.2	50.79
Ag_2O(s)	231.74	−31.05	−11.20	121.3	65.86
$AgNO_3$(s)	169.88	−129.39	−33.41	140.92	93.05
Sodium					
Na(s)	22.99	0	0	51.21	28.24
Na(g)	22.99	+107.32	+76.76	153.71	20.79
Na^+(aq)	22.99	−240.12	−261.91	59.0	46.4
NaOH(s)	40.00	−425.61	−379.49	64.46	59.54
NaCl(s)	58.44	−411.15	−384.14	72.13	50.50
NaBr(s)	102.90	−361.06	−348.98	86.82	51.38
NaI(s)	149.89	−287.78	−286.06	98.53	52.09
Sulfur					
S(s, α) (rhombic)	32.06	0	0	31.80	22.64
S(s, β) (monoclinic)	32.06	+0.33	+0.1	32.6	23.6
S(g)	32.06	+278.81	+238.25	167.82	23.673
S_2(g)	64.13	+128.37	+79.30	228.18	32.47
S^{2-}(aq)	32.06	+33.1	+85.8	−14.6	
SO_2(g)	64.06	−296.83	−300.19	248.22	39.87
SO_3(g)	80.06	−395.72	−371.06	256.76	50.67
H_2SO_4(l)	98.08	−813.99	− 690.00	156.90	138.9
H_2SO_4(aq)	98.08	−909.27	−744.53	20.1	−293
SO_4^{2-}(aq)	96.06	−909.27	−744.53	20.1	−293
HSO_4^-(aq)	97.07	−887.34	−755.91	131.8	−84

Table 2.6 (Continued)

	M/(g mol^{-1})	$\Delta_f H^\ominus$/(kJ mol^{-1})	$\Delta_f G^\ominus$/(kJ mol^{-1})	$S^\ominus_m$/(J K^{-1} mol^{-1})	$C^\ominus_{p,m}$/(J K^{-1} mol^{-1})
Sulfur (Continued)					
H_2S(g)	34.08	−20.63	−33.56	205.79	34.23
H_2S(aq)	34.08	−39.7	−27.83	121	
HS^-(aq)	33.072	−17.6	+12.08	62.08	
SF_6(g)	146.05	−1209	−1105.3	291.82	97.28
Tin					
Sn(s, β)	118.69	0	0	51.55	26.99
Sn(g)	118.69	+302.1	+267.3	168.49	20.26
Sn^{2+}(aq)	118.69	−8.8	−27.2	−17	
SnO(s)	134.69	−285.8	−256.9	56.5	44.31
SnO_2(s)	150.69	−580.7	−519.6	52.3	52.59
Xenon					
Xe(g)	131.30	0	0	169.68	20.786
Zinc					
Zn(s)	65.37	0	0	41.63	25.40
Zn(g)	65.37	+130.73	+95.14	160.98	20.79
Zn^{2+}(aq)	65.37	−153.89	−147.06	−112.1	46
ZnO(s)	81.37	−348.28	−318.30	43.64	40.25

Source: NBS

Supplementary thermochemical information

Table 2.6a Lattice enthalpies, $\Delta H^\ominus_L$/(kJ mol^{-1})

	F	Cl	Br	I
Halides				
Li	1037	852	815	761
Na	926	787	752	705
K	821	717	689	649
Rb	789	695	668	632
Cs	750	676	654	620
Ag	969	912	900	886
Be		3017		
Mg		2524		
Ca		2255		
Sr		2153		
Oxides				
MgO 3850	CaO 3461	SrO 3283	BaO 3114	
Sulfides				
MgS 3406	CaS 3119	SrS 2974	BaS 2832	

Entries refer to $MX(s) \rightarrow M^+(g) + X^-(g)$.
Data: Principally D. Cubicciotti, *J. Chem. Phys.* 31, 1646 (1959).

Table 2.6b Standard enthalpies of hydration at infinite dilution, $\Delta_{hyd}H^\ominus$/(kJ mol^{-1})

	Li^+	Na^+	K^+	Rb^+	Cs^+
F^-	−1026	−911	−828	−806	−782
Cl^-	−884	−783	−685	−664	−640
Br^-	−856	−742	−658	−637	−613
I^-	−815	−701	−617	−596	−572

Entries refer to $X^+(g) + Y^-(g) \rightarrow X^+(aq) + Y^-(aq)$.
Data: Principally J.O'M. Bockris and A.K.N. Reddy, *Modern electrochemistry*, Vol. 1. Plenum Press, New York (1970).

Table 2.6c Standard ion hydration enthalpies, $\Delta_{hyd}H^{\ominus}/(kJ\,mol^{-1})$ at 298 K

Cations						Anions							
H^+	(−1090)	Ag^+	−464	Mg^{2+}	−1920	OH^-	−460						
Li^+	−520	NH_4^+	−301	Ca^{2+}	−1650	F^-	−506	Cl^-	−364	Br^-	−337	I^-	−296
Na^+	−405			Sr^{2+}	−1480								
K^+	−321			Ba^{2+}	−1360								
Rb^+	−300			Fe^{2+}	−1950								
Cs^+	−277			Cu^{2+}	−2100								
				Zn^{2+}	−2050								
				Al^{3+}	−4690								
				Fe^{3+}	−4430								

Entries refer to $X^{\pm}(g) \rightarrow X^{\pm}(aq)$ based on $H^+(g) \rightarrow H^+(aq)$; $\Delta H^{\ominus} = -1090\,kJ\,mol^{-1}$.
Data: Principally J.O'M. Bockris and A.K.N. Reddy, *Modern electrochemistry*, Vol. 1. Plenum Press, New York (1970).

Table 2.7 Benson thermochemical groups

Group	$\Delta_f H^{\ominus}/(kJ\,mol^{-1})$	$S_m^{\ominus}/(J\,K^{-1}\,mol^{-1})$	$C_{p,m}^{\ominus}/(J\,K^{-1}\,mol^{-1})$
$C(H)_3(C)$	−42.17	127.2	25.9
$C(H)_2(C)_2$	−20.7	39.4	22.8
$C(H)(C)_3$	−6.19	−50.50	18.7
$C(C)_4$	+8.16	−146.9	18.2
$C(Cl)(H)_2(C)$	−65.7	158	37
$C(Br)(H)_2(C)$	−22	169	38
$C(I)(H)_2(C)$	+37		
$C(Cl)(H)(C)_2$	−60.2	74.1	36
$C(Br)(H)(C)_2$	−9.6	84.9	
$C(Cl)(H)(C)_3$	−53.1	−32	36
$C(Br)(H)(C)_3$		−18	39
$C(Cl)_3(C)$		210.	66.1
[O—(C)(H)] + [C—(O)(H)$_3$]	−48.1	59.5	10.5
[O—(C)(C)] + 2[C—(O)(H)$_3$]	−45.3	69.4	15.7
[C—(O)(C)(H)$_2$] + 2[C—(O)(H)$_3$]	+2.0	−20.4	−1.1

Data: S.W. Benson, *Thermochemical kinetics*. McGraw-Hill, New York (1976).

Table 3.1 Expansion coefficients, α, and isothermal compressibilities, κ_T

	$\alpha/(10^{-4}\,K^{-1})$	$\kappa_T/(10^{-6}\,atm^{-1})$
Liquids		
Benzene	12.4	92.1
Carbon tetrachloride	12.4	90.5
Ethanol	11.2	76.8
Mercury	1.82	38.7
Water	2.1	49.6
Solids		
Copper	0.501	0.735
Diamond	0.030	0.187
Iron	0.354	0.589
Lead	0.861	2.21

The values refer to 20 °C
Data: AIP(α), KL(κ_T).

Table 3.2 Inversion temperatures, normal freezing and boiling points, and Joule–Thomson coefficients at 1 atm and 298 K

	T_I/K	T_f/K	T_b/K	$\mu_{JT}/(K\,atm^{-1})$
Air	603			0.189 at 50°C
Argon	723	83.8	87.3	
Carbon dioxide	1500	194.7s		1.11 at 300 K
Helium	40		4.22	−0.062
Hydrogen	202	14.0	20.3	−0.03
Krypton	1090	116.6	120.8	
Methane	968	90.6	111.6	
Neon	231	24.5	27.1	
Nitrogen	621	63.3	77.4	0.27
Oxygen	764	54.8	90.2	0.31

s: sublimes
Data: AIP, JL, and M.W. Zemansky, *Heat and thermodynamics*. McGraw-Hill, New York (1957).

Table 4.1 Standard entropies (and temperatures) of phase transitions at 1 atm, $\Delta_{trs}S^{\ominus}/(J\,K^{-1}\,mol^{-1})$

	Fusion (at T_f)	Vaporization (at T_b)
Ar	14.17 (at 83.8 K)	74.53 (at 87.3 K)
Br_2	39.76 (at 265.9 K)	88.61 (at 332.4 K)
C_6H_6	38.00 (at 278.6 K)	87.19 (at 353.2 K)
CH_3COOH	40.4 (at 289.8 K)	61.9 (at 391.4 K)
CH_3OH	18.03 (at 175.2 K)	104.6 (at 337.2 K)
Cl_2	37.22 (at 172.1 K)	85.38 (at 239.0 K)
H_2	8.38 (at 14.0 K)	44.96 (at 20.38 K)
H_2O	22.00 (at 273.2 K)	109.0 (at 373.2 K)
H_2S	12.67 (at 187.6 K)	87.75 (at 212.0 K)
He	4.8 (at 1.8 K and 30 bar)	19.9 (at 4.22 K)
N_2	11.39 (at 63.2 K)	75.22 (at 77.4 K)
NH_3	28.93 (at 195.4 K)	97.41 (at 239.73 K)
O_2	8.17 (at 54.4 K)	75.63 (at 90.2 K)

Data: AIP

Table 4.2 Standard entropies of vaporization of liquids at their normal boiling point

	$\Delta_{vap}H^{\ominus}/(kJ\,mol^{-1})$	$\theta_b/°C$	$\Delta_{vap}S^{\ominus}/(J\,K^{-1}\,mol^{-1})$
Benzene	30.8	80.1	+87.2
Carbon disulfide	26.74	46.25	+83.7
Carbon tetrachloride	30.00	76.7	+85.8
Cyclohexane	30.1	80.7	+85.1
Decane	38.75	174	+86.7
Dimethyl ether	21.51	−23	+86
Ethanol	38.6	78.3	+110.0
Hydrogen sulfide	18.7	−60.4	+87.9
Mercury	59.3	356.6	+94.2
Methane	8.18	−161.5	+73.2
Methanol	35.21	65.0	+104.1
Water	40.7	100.0	+109.1

Data: JL

Table 4.3 Standard Third-Law entropies at 298 K: see Tables 2.5 and 2.6

Table 4.4 Standard Gibbs energies of formation at 298 K: see Tables 2.5 and 2.6

Table 5.2 The fugacity coefficient of nitrogen at 273 K

p/atm	ϕ	p/atm	ϕ
1	0.99955	300	1.0055
10	0.9956	400	1.062
50	0.9812	600	1.239
100	0.9703	800	1.495
150	0.9672	1000	1.839
200	0.9721		

Data: LR

Table 6.1 Surface tensions of liquids at 293 K

	$\gamma/(\mathrm{mN\,m^{-1}})$
Benzene	28.88
Carbon tetrachloride	27.0
Ethanol	22.8
Hexane	18.4
Mercury	472
Methanol	22.6
Water	72.75
	72.0 at 25°C
	58.0 at 100°C

Data: KL

Table 7.1 Henry's law constants for gases at 298 K, K/Torr

	Water	Benzene
CH_4	3.14×10^5	4.27×10^5
CO_2	1.25×10^6	8.57×10^4
H_2	5.34×10^7	2.75×10^6
N_2	6.51×10^7	1.79×10^6
O_2	3.30×10^7	

Data: F. Daniels and R.A. Alberty, *Physical chemistry*. Wiley, New York (1980).

Table 7.2 Cryoscopic and ebullioscopic constants

	$K_f/(\mathrm{K\,kg\,mol^{-1}})$	$K_b/(\mathrm{K\,kg\,mol^{-1}})$
Acetic acid	3.90	3.07
Benzene	5.12	2.53
Camphor	40	
Carbon disulfide	3.8	2.37
Carbon tetrachloride	30	4.95
Naphthalene	6.94	5.8
Phenol	7.27	3.04
Water	1.86	0.51

Data: KL

Table 9.1 Acidity constants for aqueous solution at 298 K. (a) In order of acid strength

Acid	HA	A^-	K_a	pK_a
Hydroiodic	HI	I^-	10^{11}	−11
Perchloric	$HClO_4$	ClO_4^-	10^{10}	−10
Hydrobromic	HBr	Br^-	10^9	−9
Hydrochloric	HCl	Cl^-	10^7	−7
Sulfuric	H_2SO_4	HSO_4^-	10^2	−2
Hydronium ion	H_3O^+	H_2O	1	0.0
Oxalic	$(COOH)_2$	$HOOCCO_2^-$	5.9×10^{-2}	1.23
Sulfurous	H_2SO_3	HSO_3^-	1.5×10^{-2}	1.81
Hydrogensulfate ion	HSO_4^-	SO_4^{2-}	1.2×10^{-2}	1.92
Phosphoric	H_3PO_4	$H_2PO_4^-$	7.5×10^{-3}	2.12
Hydrofluoric	HF	F^-	3.5×10^{-4}	3.45
Formic	HCOOH	HCO_2^-	1.8×10^{-4}	3.75
Lactic	$CH_3CH(OH)COOH$	$CH_3CH(OH)CO_2^-$	1.4×10^{-4}	3.86
Hydrogenoxalate ion	$HOOCCO_2^-$	$(CO_2)_2^{2-}$	6.5×10^{-5}	4.19
Anilinium ion	$C_6H_5NH_3^+$	$C_6H_5NH_2$	2.3×10^{-5}	4.63
Acetic (ethanoic)	CH_3COOH	$CH_3CO_2^-$	1.8×10^{-5}	4.75
Butanoic	C_3H_7COOH	$C_3H_7CO_2^-$	1.5×10^{-5}	4.82
Propanoic	C_2H_5COOH	$C_2H_5CO_2^-$	1.4×10^{-5}	4.87
Pyridinium ion	$HC_5H_5N^+$	C_5H_5N	5.6×10^{-6}	5.25
Carbonic	H_2CO_3	HCO_3^-	4.3×10^{-7}	6.37
Hydrogen sulfide	H_2S	HS^-	9.1×10^{-8}	7.04
Dihydrogenphosphate ion	$H_2PO_4^-$	HPO_4^{2-}	6.2×10^{-8}	7.21
Hypochlorous	HClO	ClO^-	3.0×10^{-8}	7.53
Hydrazinium ion	$NH_2NH_3^+$	NH_2NH_2	5.9×10^{-9}	8.23
Hypobromous	HBrO	BrO^-	2.0×10^{-9}	8.69
Boric	$B(OH)_3$	$B(OH)_4^-$	7.2×10^{-10}	9.14
Ammonium ion	NH_4^+	NH_3	5.6×10^{-10}	9.25
Hydrogen cyanide	HCN	CN^-	4.9×10^{-10}	9.31
Glycinium ion	NH_2CH_2COOH	$NH_2CH_2CO_2^-$	1.7×10^{-10}	9.78
Trimethylammonium ion	$(CH_3)_3NH^+$	$(CH_3)_3N$	1.6×10^{-10}	9.81
Phenol	C_6H_5OH	$C_6H_5O^-$	1.3×10^{-10}	9.89
Hydrogencarbonate ion	HCO_3^-	CO_3^{2-}	5.6×10^{-11}	10.25
Hypoiodous	HIO	IO^-	2.3×10^{-11}	10.64
Methylammonium ion	$CH_3NH_3^+$	CH_3NH_2	2.2×10^{-11}	10.66
Dimethylammonium ion	$(CH_3)_2NH_2^+$	$(CH_3)_2NH$	1.9×10^{-11}	10.73
Triethylammonium ion	$(C_2H_5)_3NH^+$	$(C_2H_5)_3N$	1.7×10^{-11}	10.76
Ethylammonium ion	$C_2H_5NH_3^+$	$C_2H_5NH_2$	1.6×10^{-11}	10.81
Diethylammonium ion	$(C_2H_5)_2NH_2^+$	$(C_2H_5)_2NH$	1.0×10^{-11}	10.99
Hydrogenarsenate ion	$HAsO_4^{2-}$	AsO_4^{3-}	3.0×10^{-12}	11.53
Hydrogensulfide ion	HS^-	S^{2-}	1.1×10^{-12}	11.96
Hydrogenphosphate ion	HPO_4^{2-}	PO_4^{3-}	2.2×10^{-13}	12.67

Data: Principally HCP

Table 9.1 Acidity constants for aqueous solution at 298 K. (b) In alphabetical order of acid

Acid	HA	A^-	K_a	pK_a
Acetic	CH_3COOH	$CH_3CO_2^-$	1.8×10^{-5}	4.75
Ammonium ion	NH_4^+	NH_3	5.6×10^{-10}	9.25
Anilinium ion	$C_6H_5NH_3^+$	$C_6H_5NH_2$	2.3×10^{-5}	4.63
Boric	$B(OH)_3$	$B(OH)_4^-$	7.2×10^{-10}	9.14
Butanoic	C_3H_7COOH	$C_3H_7CO_2^-$	1.5×10^{-5}	4.82
Carbonic	H_2CO_3	HCO_3^-	4.3×10^{-7}	6.37
Diethylammonium ion	$(C_2H_5)_2NH_2^+$	$(C_2H_5)_2NH$	1.0×10^{-11}	10.99
Dihydrogenphosphate ion	$H_2PO_4^-$	HPO_4^{2-}	6.2×10^{-8}	7.21
Dimethylammonium ion	$(CH_3)_2NH_2^+$	$(CH_3)_2NH$	1.9×10^{-11}	10.73
Ethylammonium ion	$C_2H_5NH_3^+$	$C_2H_5NH_2$	1.6×10^{-11}	10.81
Formic	$HCOOH$	HCO_2^-	1.8×10^{-4}	3.75
Glycinium ion	NH_2CH_2COOH	$NH_2CH_2CO_2^-$	1.7×10^{-10}	9.78
Hydrazinium ion	$NH_2NH_3^+$	NH_2NH_2	5.9×10^{-9}	8.23
Hydroiodic	HI	I^-	10^{11}	−11
Hydrobromic	HBr	Br^-	10^{9}	−9
Hydrochloric	HCl	Cl^-	10^{7}	−7
Hydrofluoric	HF	F^-	3.5×10^{-4}	3.45
Hydrogenarsenate ion	$HAsO_4^{2-}$	AsO_4^{3-}	3.0×10^{-12}	11.53
Hydrogencarbonate ion	HCO_3^-	CO_3^{2-}	4.8×10^{-11}	10.32
Hydrogen cyanide	HCN	CN^-	4.9×10^{-10}	9.31
Hydrogenoxalate ion	$HOOCCO_2^-$	$(CO_2)_2^{2-}$	6.5×10^{-5}	4.19
Hydrogenphosphate ion	HPO_4^{2-}	PO_4^{3-}	2.2×10^{-13}	12.67
Hydrogensulfate ion	HSO_4^-	SO_4^{2-}	1.2×10^{-2}	1.92
Hydrogen sulfide	H_2S	HS^-	9.1×10^{-8}	7.04
Hydrogensulfide ion	HS^-	S^{2-}	1.1×10^{-12}	11.96
Hydronium ion	H_3O^+	H_2O	1	0.0
Hypobromous	$HBrO$	BrO^-	2.0×10^{-9}	8.69
Hypochlorous	$HClO$	ClO^-	3.0×10^{-8}	7.53
Hypoiodous	HIO	IO^-	2.3×10^{-11}	10.64
Lactic	$CH_3CH(OH)COOH$	$CH_3CH(OH)CO_2^-$	1.4×10^{-4}	3.86
Methylammonium ion	$CH_3NH_3^+$	CH_3NH_2	2.2×10^{-11}	10.66
Oxalic	$(COOH)_2$	$HOOCCO_2^-$	5.9×10^{-2}	1.23
Perchloric	$HClO_4$	ClO_4^-	10^{10}	−10
Phenol	C_6H_5OH	$C_6H_5O^-$	1.3×10^{-10}	9.89
Phosphoric	H_3PO_4	$H_2PO_4^-$	7.5×10^{-3}	2.12
Propanoic	C_2H_5COOH	$C_2H_5CO_2^-$	1.4×10^{-5}	4.87
Pyridinium ion	$HC_5H_5N^+$	C_5H_5N	5.6×10^{-6}	5.25
Sulfuric	H_2SO_4	HSO_4^-	10^{2}	−2
Sulfurous	H_2SO_3	HSO_3^-	1.5×10^{-2}	1.81
Triethylammonium ion	$(C_2H_5)_3NH^+$	$(C_2H_5)_3N$	1.7×10^{-11}	10.76
Trimethylammonium ion	$(CH_3)_3NH^+$	$(CH_3)_3N$	1.6×10^{-10}	9.81

Table 10.1 Standard thermodynamic functions of ions in solution at 298 K. See Table 2.6

Table 10.2 Relative permittivities (dielectric constants) at 298 K

Nonpolar molecules		Polar molecules	
Methane (at −173°C)	1.70	Water	78.54 80.37 at 20°C
Carbon tetrachloride	2.228	Ammonia	16.9 22.4 at −33°C
Cyclohexane	2.015	Hydrogen sulfide	9.26 at −85°C
Benzene	2.274	Methanol	32.63
		Ethanol	24.30
		Nitrobenzene	34.82

Data: HCP

Table 10.3 Standard molar entropies of ions in aqueous solution at 298 K. See Table 2.6

Table 10.5 Mean activity coefficients in water at 298 K

$b/b^{\ominus}$	HCl	KCl	$CaCl_2$	H_2SO_4	$LaCl_3$	$In_2(SO_4)_3$
0.001	0.966	0.966	0.888	0.830	0.790	
0.005	0.929	0.927	0.789	0.639	0.636	0.16
0.01	0.905	0.902	0.732	0.544	0.560	0.11
0.05	0.830	0.816	0.584	0.340	0.388	0.035
0.10	0.798	0.770	0.524	0.266	0.356	0.025
0.50	0.769	0.652	0.510	0.155	0.303	0.014
1.00	0.811	0.607	0.725	0.131	0.387	
2.00	1.011	0.577	1.554	0.125	0.954	

Data: RS, HCP, and S. Glasstone, *Introduction to electrochemistry*. Van Nostrand (1942).

Table 10.7 Standard potentials at 298 K. (a) In electrochemical order

Reduction half-reaction	$E^\ominus$/V	Reduction half-reaction	$E^\ominus$/V
Strongly oxidizing			
$H_4XeO_6 + 2H^+ + 2e^- \rightarrow XeO_3 + 3H_2O$	+3.0	$Cu^{2+} + e^- \rightarrow Cu^+$	+0.16
$F_2 + 2e^- \rightarrow 2F^-$	+2.87	$Sn^{4+} + 2e^- \rightarrow Sn^{2+}$	+0.15
$O_3 + 2H^+ + 2e^- \rightarrow O_2 + H_2O$	+2.07	$AgBr + e^- \rightarrow Ag + Br^-$	+0.07
$S_2O_8^{2-} + 2e^- \rightarrow 2SO_4^{2-}$	+2.05	$Ti^{4+} + e^- \rightarrow Ti^{3+}$	0.00
$Ag^{2+} + e^- \rightarrow Ag^+$	+1.98	$2H^+ + 2e^- \rightarrow H_2$	0, by definition
$Co^{3+} + e^- \rightarrow Co^{2+}$	+1.81	$Fe^{3+} + 3e^- \rightarrow Fe$	−0.04
$H_2O_2 + 2H^+ + 2e^- \rightarrow 2H_2O$	+1.78	$O_2 + H_2O + 2e^- \rightarrow HO_2^- + OH^-$	−0.08
$Au^+ + e^- \rightarrow Au$	+1.69	$Pb^{2+} + 2e^- \rightarrow Pb$	−0.13
$Pb^{4+} + 2e^- \rightarrow Pb^{2+}$	+1.67	$In^+ + e^- \rightarrow In$	−0.14
$2HClO + 2H^+ + 2e^- \rightarrow Cl_2 + 2H_2O$	+1.63	$Sn^{2+} + 2e^- \rightarrow Sn$	−0.14
$Ce^{4+} + e^- \rightarrow Ce^{3+}$	+1.61	$AgI + e^- \rightarrow Ag + I^-$	−0.15
$2HBrO + 2H^+ + 2e^- \rightarrow Br_2 + 2H_2O$	+1.60	$Ni^{2+} + 2e^- \rightarrow Ni$	−0.23
$MnO_4^- + 8H^+ + 5e^- \rightarrow Mn^{2+} + 4H_2O$	+1.51	$Co^{2+} + 2e^- \rightarrow Co$	−0.28
$Mn^{3+} + e^- \rightarrow Mn^{2+}$	+1.51	$In^{3+} + 3e^- \rightarrow In$	−0.34
$Au^{3+} + 3e^- \rightarrow Au$	+1.40	$Tl^+ + e^- \rightarrow Tl$	−0.34
$Cl_2 + 2e^- \rightarrow 2Cl^-$	+1.36	$PbSO_4 + 2e^- \rightarrow Pb + SO_4^{2-}$	−0.36
$Cr_2O_7^{2-} + 14H^+ + 6e^- \rightarrow 2Cr^{3+} + 7H_2O$	+1.33	$Ti^{3+} + e^- \rightarrow Ti^{2+}$	−0.37
$O_3 + H_2O + 2e^- \rightarrow O_2 + 2OH^-$	+1.24	$Cd^{2+} + 2e^- \rightarrow Cd$	−0.40
$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$	+1.23	$In^{2+} + e^- \rightarrow In^+$	−0.40
$ClO_4^- + 2H^+ + 2e^- \rightarrow ClO_3^- + H_2O$	+1.23	$Cr^{3+} + e^- \rightarrow Cr^{2+}$	−0.41
$MnO_2 + 4H^+ + 2e^- \rightarrow Mn^{2+} + 2H_2O$	+1.23	$Fe^{2+} + 2e^- \rightarrow Fe$	−0.44
$Br_2 + 2e^- \rightarrow 2Br^-$	+1.09	$In^{3+} + 2e^- \rightarrow In^+$	−0.44
$Pu^{4+} + e^- \rightarrow Pu^{3+}$	+0.97	$S + 2e^- \rightarrow S^{2-}$	−0.48
$NO_3^- + 4H^+ + 3e^- \rightarrow NO + 2H_2O$	+0.96	$In^{3+} + e^- \rightarrow In^{2+}$	−0.49
$2Hg^{2+} + 2e^- \rightarrow Hg_2^{2+}$	+0.92	$U^{4+} + e^- \rightarrow U^{3+}$	−0.61
$ClO^- + H_2O + 2e^- \rightarrow Cl^- + 2OH^-$	+0.89	$Cr^{3+} + 3e^- \rightarrow Cr$	−0.74
$Hg^{2+} + 2e^- \rightarrow Hg$	+0.86	$Zn^{2+} + 2e^- \rightarrow Zn$	−0.76
$NO_3^- + 2H^+ + e^- \rightarrow NO_2 + H_2O$	+0.80	$Cd(OH)_2 + 2e^- \rightarrow Cd + 2OH^-$	−0.81
$Ag^+ + e^- \rightarrow Ag$	+0.80	$2H_2O + 2e^- \rightarrow H_2 + 2OH^-$	−0.83
$Hg_2^{2+} + 2e^- \rightarrow 2Hg$	+0.79	$Cr^{2+} + 2e^- \rightarrow Cr$	−0.91
$Fe^{3+} + e^- \rightarrow Fe^{2+}$	+0.77	$Mn^{2+} + 2e^- \rightarrow Mn$	−1.18
$BrO^- + H_2O + 2e^- \rightarrow Br^- + 2OH^-$	+0.76	$V^{2+} + 2e^- \rightarrow V$	−1.19
$Hg_2SO_4 + 2e^- \rightarrow 2Hg + SO_4^{2-}$	+0.62	$Ti^{2+} + 2e^- \rightarrow Ti$	−1.63
$MnO_4^{2-} + 2H_2O + 2e^- \rightarrow MnO_2 + 4OH^-$	+0.60	$Al^{3+} + 3e^- \rightarrow Al$	−1.66
$MnO_4^- + e^- \rightarrow MnO_4^{2-}$	+0.56	$U^{3+} + 3e^- \rightarrow U$	−1.79
$I_2 + 2e^- \rightarrow 2I^-$	+0.54	$Sc^{3+} + 3e^- \rightarrow Sc$	−2.09
$Cu^+ + e^- \rightarrow Cu$	+0.52	$Mg^{2+} + 2e^- \rightarrow Mg$	−2.36
$I_3^- + 2e^- \rightarrow 3I^-$	+0.53	$Ce^{3+} + 3e^- \rightarrow Ce$	−2.48
$NiOOH + H_2O + e^- \rightarrow Ni(OH)_2 + OH^-$	+0.49	$La^{3+} + 3e^- \rightarrow La$	−2.52
$Ag_2CrO_4 + 2e^- \rightarrow 2Ag + CrO_4^{2-}$	+0.45	$Na^+ + e^- \rightarrow Na$	−2.71
$O_2 + 2H_2O + 4e^- \rightarrow 4OH^-$	+0.40	$Ca^{2+} + 2e^- \rightarrow Ca$	−2.87
$ClO_4^- + H_2O + 2e^- \rightarrow ClO_3^- + 2OH^-$	+0.36	$Sr^{2+} + 2e^- \rightarrow Sr$	−2.89
$[Fe(CN)_6]^{3-} + e^- \rightarrow [Fe(CN)_6]^{4-}$	+0.36	$Ba^{2+} + 2e^- \rightarrow Ba$	−2.91
$Cu^{2+} + 2e^- \rightarrow Cu$	+0.34	$Ra^{2+} + 2e^- \rightarrow Ra$	−2.92
$Hg_2Cl_2 + 2e^- \rightarrow 2Hg + 2Cl^-$	+0.27	$Cs^+ + e^- \rightarrow Cs$	−2.92
$AgCl + e^- \rightarrow Ag + Cl^-$	+0.22	$Rb^+ + e^- \rightarrow Rb$	−2.93
$Bi^{3+} + 3e^- \rightarrow Bi$	+0.20	$K^+ + e^- \rightarrow K$	−2.93

Table 10.7 Standard electrode potentials at 298 K. (b) In alphabetical order

Reduction half-reaction	$E^{\ominus}$/V	Reduction half-reaction	$E^{\ominus}$/V
$Li^+ + e^- \rightarrow Li$	−3.05	$I_2 + 2e^- \rightarrow 2I^-$	+0.54
$Ag^+ + e^- \rightarrow Ag$	+0.80	$I_3^- + 2e^- \rightarrow 3I^-$	+0.53
$Ag^{2+} + e^- \rightarrow Ag^+$	+1.98	$In^+ + e^- \rightarrow In$	−0.14
$AgBr + e^- \rightarrow Ag + Br^-$	+0.0713	$In^{2+} + e^- \rightarrow In^+$	−0.40
$AgCl + e^- \rightarrow Ag + Cl^-$	+0.22	$In^{3+} + 2e^- \rightarrow In^+$	−0.44
$Ag_2CrO_4 + 2e^- \rightarrow 2Ag + CrO_4^{2-}$	+0.45	$In^{3+} + 3e^- \rightarrow In$	−0.34
$AgF + e^- \rightarrow Ag + F^-$	+0.78	$In^{3+} + e^- \rightarrow In^{2+}$	−0.49
$AgI + e^- \rightarrow Ag + I^-$	−0.15	$K^+ + e^- \rightarrow K$	−2.93
$Al^{3+} + 3e^- \rightarrow Al$	−1.66	$La^{3+} + 3e^- \rightarrow La$	−2.52
$Au^+ + e^- \rightarrow Au$	+1.69	$Li^+ + e^- \rightarrow Li$	−3.05
$Au^{3+} + 3e^- \rightarrow Au$	+1.40	$Mg^{2+} + 2e^- \rightarrow Mg$	−2.36
$Ba^{2+} + 2e^- \rightarrow Ba$	−2.91	$Mn^{2+} + 2e^- \rightarrow Mn$	−1.18
$Be^{2+} + 2e^- \rightarrow Be$	−1.85	$Mn^{3+} + e^- \rightarrow Mn^{2+}$	+1.51
$Bi^{3+} + 3e^- \rightarrow Bi$	+0.20	$MnO_2 + 4H^+ + 2e^- \rightarrow Mn^{2+} + 2H_2O$	+1.23
$Br_2 + 2e^- \rightarrow 2Br^-$	+1.09	$MnO_4^- + 8H^+ + 5e^- \rightarrow Mn^{2+} + 4H_2O$	+1.51
$BrO^- + H_2O + 2e^- \rightarrow Br^- + 2OH^-$	+0.76	$MnO_4^- + e^- \rightarrow MnO_4^{2-}$	+0.56
$Ca^{2+} + 2e^- \rightarrow Ca$	−2.87	$MnO_4^{2-} + 2H_2O + 2e^- \rightarrow MnO_2 + 4OH^-$	+0.60
$Cd(OH)_2 + 2e^- \rightarrow Cd + 2OH^-$	−0.81	$Na^+ + e^- \rightarrow Na$	−2.71
$Cd^{2+} + 2e^- \rightarrow Cd$	−0.40	$Ni^{2+} + 2e^- \rightarrow Ni$	−0.23
$Ce^{3+} + 3e^- \rightarrow Ce$	−2.48	$NiOOH + H_2O + e^- \rightarrow Ni(OH)_2 + OH^-$	+0.49
$Ce^{4+} + e^- \rightarrow Ce^{3+}$	+1.61	$NO_3^- + 2H^+ + e^- \rightarrow NO_2 + H_2O$	−0.80
$Cl_2 + 2e^- \rightarrow 2Cl^-$	+1.36	$NO_3^- + 4H^+ + 3e^- \rightarrow NO + 2H_2O$	+0.96
$ClO^- + H_2O + 2e^- \rightarrow Cl^- + 2OH^-$	+0.89	$NO_3^- + H_2O + 2e^- \rightarrow NO_2^- + 2OH^-$	+0.10
$ClO_4^- + 2H^+ + 2e^- \rightarrow ClO_3^- + H_2O$	+1.23	$O_2 + 2H_2O + 4e^- \rightarrow 4OH^-$	+0.40
$ClO_4^- + H_2O + 2e^- \rightarrow ClO_3^- + 2OH^-$	+0.36	$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$	+1.23
$Co^{2+} + 2e^- \rightarrow Co$	−0.28	$O_2 + e^- \rightarrow O_2^-$	−0.56
$Co^{3+} + e^- \rightarrow Co^{2+}$	+1.81	$O_2 + H_2O + 2e^- \rightarrow HO_2^- + OH^-$	−0.08
$Cr^{2+} + 2e^- \rightarrow Cr$	−0.91	$O_3 + 2H^+ + 2e^- \rightarrow O_2 + H_2O$	+2.07
$Cr_2O_7^{2-} + 14H^+ + 6e^- \rightarrow 2Cr^{3+} + 7H_2O$	+1.33	$O_3 + H_2O + 2e^- \rightarrow O_2 + 2OH^-$	+1.24
$Cr^{3+} + 3e^- \rightarrow Cr$	−0.74	$Pb^{2+} + 2e^- \rightarrow Pb$	−0.13
$Cr^{3+} + e^- \rightarrow Cr^{2+}$	−0.41	$Pb^{4+} + 2e^- \rightarrow Pb^{2+}$	+1.67
$Cs^+ + e^- \rightarrow Cs$	−2.92	$PbSO_4 + 2e^- \rightarrow Pb + SO_4^{2-}$	−0.36
$Cu^+ + e^- \rightarrow Cu$	+0.52	$Pt^{2+} + 2e^- \rightarrow Pt$	+1.20
$Cu^{2+} + 2e^- \rightarrow Cu$	+0.34	$Pu^{4+} + e^- \rightarrow Pu^{3+}$	+0.97
$Cu^{2+} + e^- \rightarrow Cu^+$	+0.16	$Ra^{2+} + 2e^- \rightarrow Ra$	−2.92
$F_2 + 2e^- \rightarrow 2F^-$	+2.87	$Rb^+ + e^- \rightarrow Rb$	−2.93
$Fe^{2+} + 2e^- \rightarrow Fe$	−0.44	$S + 2e^- \rightarrow S^{2-}$	−0.48
$Fe^{3+} + 3e^- \rightarrow Fe$	−0.04	$S_2O_8^{2-} + 2e^- \rightarrow 2SO_4^{2-}$	+2.05
$Fe^{3+} + e^- \rightarrow Fe^{2+}$	+0.77	$Sc^{3+} + 3e^- \rightarrow Sc$	−2.09
$[Fe(CN)_6]^{3-} + e^- \rightarrow [Fe(CN)_6]^{4-}$	+0.36	$Sn^{2+} + 2e^- \rightarrow Sn$	−0.14
$2H^+ + 2e^- \rightarrow H_2$	0, by definition	$Sn^{4+} + 2e^- \rightarrow Sn^{2+}$	+0.15
$2H_2O + 2e^- \rightarrow H_2 + 2OH^-$	−0.83	$Sr^{2+} + 2e^- \rightarrow Sr$	−2.89
$2HBrO + 2H^+ + 2e^- \rightarrow Br_2 + 2H_2O$	+1.60	$Ti^{2+} + 2e^- \rightarrow Ti$	−1.63
$2HClO + 2H^+ + 2e^- \rightarrow Cl_2 + 2H_2O$	+1.63	$Ti^{3+} + e^- \rightarrow Ti^{2+}$	−0.37
$H_2O_2 + 2H^+ + 2e^- \rightarrow 2H_2O$	+1.78	$Ti^{4+} + e^- \rightarrow Ti^{3+}$	0.00
$H_4XeO_6 + 2H^+ + 2e^- \rightarrow XeO_3 + 3H_2O$	+3.0	$Tl^+ + e^- \rightarrow Tl$	−0.34
$Hg_2^{2+} + 2e^- \rightarrow 2Hg$	+0.79	$U^{3+} + 3e^- \rightarrow U$	−1.79
$Hg_2Cl_2 + 2e^- \rightarrow 2Hg + 2Cl^-$	+0.27	$U^{4+} + e^- \rightarrow U^{3+}$	−0.61
$Hg^{2+} + 2e^- \rightarrow Hg$	+0.86	$V^{2+} + 2e^- \rightarrow V$	−1.19
$2Hg^{2+} + 2e^- \rightarrow Hg_2^{2+}$	+0.92	$V^{3+} + e^- \rightarrow V^{2+}$	−0.26
$Hg_2SO_4 + 2e^- \rightarrow 2Hg + SO_4^{2-}$	+0.62	$Zn^{2+} + 2e^- \rightarrow Zn$	−0.76

Table 12.2 The error function

z	erf z	z	erf z
0	0	0.45	0.475 48
0.01	0.011 28	0.50	0.520 50
0.02	0.022 56	0.55	0.563 32
0.03	0.033 84	0.60	0.603 86
0.04	0.045 11	0.65	0.642 03
0.05	0.056 37	0.70	0.677 80
0.06	0.067 62	0.75	0.711 16
0.07	0.078 86	0.80	0.742 10
0.08	0.090 08	0.85	0.770 67
0.09	0.101 28	0.90	0.796 91
0.10	0.112 46	0.95	0.820 89
0.15	0.168 00	1.00	0.842 70
0.20	0.222 70	1.20	0.910 31
0.25	0.276 32	1.40	0.952 28
0.30	0.328 63	1.60	0.976 35
0.35	0.379 38	1.80	0.989 09
0.40	0.428 39	2.00	0.995 32

Data: AS

Table 13.3 Screening constants for atoms; values of $Z_{eff} = Z - \sigma$ for neutral ground-state atoms

	H							He
1s	1							1.6875
	Li	Be	B	C	N	O	F	Ne
1s	2.6906	3.6848	4.6795	5.6727	6.6651	7.6579	8.6501	9.6421
2s	1.2792	1.9120	2.5762	3.2166	3.8474	4.4916	5.1276	5.7584
2p			2.4214	3.1358	3.8340	4.4532	5.1000	5.7584
	Na	Mg	Al	Si	P	S	Cl	Ar
1s	10.6259	11.6089	11910	13.5754	14.5578	15.5409	16.5239	17.5075
2s	6.5714	7.3920	8.2136	9.0200	9.8250	10.6288	11.4304	12.2304
2p	6.8018	7.8258	8.9634	9.9450	10.9612	11.9770	12.9932	14.0082
3s	2.5074	3.3075	4.1172	4.9032	5.6418	6.3669	7.0683	7.7568
3p			4.0656	4.2852	4.8864	5.4819	6.1161	6.7641

Data: E. Clementi and D.L. Raimondi, *Atomic screening constants from SCF functions.* IBM Res. Note NJ-27 (1963).

Table 13.4 Ionization energies, $I_i/(\text{kJ mol}^{-1})$

H							He
1312.0							2372.3
							5250.4
Li	Be	B	C	N	O	F	Ne
513.3	899.4	800.6	1086.2	1402.3	1313.9	1681	2080.6
7298.0	1757.1	2427	2352	2856.1	3388.2	3374	3952.2
Na	Mg	Al	Si	P	S	Cl	Ar
495.8	737.7	577.4	786.5	1011.7	999.6	1251.1	1520.4
4562.4	1450.7	1816.6	1577.1	1903.2	2251	2297	2665.2
		2744.6		2912			
K	Ca	Ga	Ge	As	Se	Br	Kr
418.8	589.7	578.8	762.1	947.0	940.9	1139.9	1350.7
3051.4	1145	1979	1537	1798	2044	2104	2350
		2963	2735				
Rb	Sr	In	Sn	Sb	Te	I	Xe
403.0	549.5	558.3	708.6	833.7	869.2	1008.4	1170.4
2632	1064.2	1820.6	1411.8	1794	1795	1845.9	2046
		2704	2943.0	2443			
Cs	Ba	Tl	Pb	Bi	Po	At	Rn
375.5	502.8	589.3	715.5	703.2	812	930	1037
2420	965.1	1971.0	1450.4	1610			
		2878	3081.5	2466			

Data: E

Table 13.5 Electron affinities, $E_{ea}/(\text{kJ mol}^{-1})$

H							He
72.8							−21
Li	Be	B	C	N	O	F	Ne
59.8	⩽0	23	122.5	−7	141	322	−29
					−844		
Na	Mg	Al	Si	P	S	Cl	Ar
52.9	⩽0	44	133.6	71.7	200.4	348.7	−35
					−532		
K	Ca	Ga	Ge	As	Se	Br	Kr
48.3	2.37	36	116	77	195.0	324.5	−39
Rb	Sr	In	Sn	Sb	Te	I	Xe
46.9	5.03	34	121	101	190.2	295.3	−41
Cs	Ba	Tl	Pb	Bi	Po	At	Rn
45.5	13.95	30	35.2	101	186	270	−41

Data: E

Table 14.2 Bond lengths, R_e/pm

(a) Bond lengths in specific molecules

Br_2	228.3
Cl_2	198.75
CO	112.81
F_2	141.78
H_2^+	106
H_2	74.138
HBr	141.44
HCl	127.45
HF	91.680
HI	160.92
N_2	109.76
O_2	120.75

(b) Mean bond lengths from covalent radii*

H	37						
C	77(1)	N	74(1)	O	66(1)	F	64
	67(2)		65(2)		57(2)		
	60(3)						
Si	118	P	110	S	104(1)	Cl	99
					95(2)		
Ge	122	As	121	Se	104	Br	114
		Sb	141	Te	137	I	133

*Values are for single bonds except where indicated otherwise (values in parentheses). The length of an A–B covalent bond (of given order) is the sum of the corresponding covalent radii.

Table 14.3a Bond dissociation enthalpies, $\Delta H^\ominus$(A—B)/(kJ mol^{-1}) at 298 K

Diatomic molecules

H—H	436	F—F	155	Cl—Cl	242	Br—Br	193	I—I	151
O=O	497	C=O	1076	N≡N	945				
H—O	428	H—F	565	H—Cl	431	H—Br	366	H—I	299

Polyatomic molecules

$H—CH_3$	435	$H—NH_2$	460	H—OH	492	$H—C_6H_5$	469
$H_3C—CH_3$	368	$H_2C=CH_2$	720	HC≡CH	962		
$HO—CH_3$	377	$Cl—CH_3$	352	$Br—CH_3$	293	$I—CH_3$	237
O=CO	531	HO—OH	213	$O_2N—NO_2$	54		

Data: HCP, KL

Table 14.3b Mean bond enthalpies, $\Delta H^{\ominus}(A—B)/(kJ\,mol^{-1})$

	H	C	N	O	F	Cl	Br	I	S	P	Si
H	436										
C	412	348(i)									
		612(ii)									
		838(iii)									
		518(a)									
N	388	305(i)	163(i)								
		613(ii)	409(ii)								
		890(iii)	946(iii)								
O	463	360(i)	157	146(i)							
		743(ii)		497(ii)							
F	565	484	270	185	155						
Cl	431	338	200	203	254	242					
Br	366	276				219	193				
I	299	238				210	178	151			
S	338	259			496	250	212		264		
P	322									201	
Si	318		374	466							226

(i) Single bond, (ii) double bond, (iii) triple bond, (a) aromatic.
Data: HCP and L. Pauling, *The nature of the chemical bond.* Cornell University Press (1960).

Table 14.4 Pauling (*italics*) and Mulliken electronegativities

H							He
2.20							
3.06							
Li	Be	B	C	N	O	F	Ne
0.98	*1.57*	*2.04*	*2.55*	*3.04*	*3.44*	*3.98*	
1.28	1.99	1.83	2.67	3.08	3.22	4.43	4.60
Na	Mg	Al	Si	P	S	Cl	Ar
0.93	*1.31*	*1.61*	*1.90*	*2.19*	*2.58*	*3.16*	
1.21	1.63	1.37	2.03	2.39	2.65	3.54	3.36
K	Ca	Ga	Ge	As	Se	Br	Kr
0.82	*1.00*	*1.81*	*2.01*	*2.18*	*2.55*	*2.96*	*3.0*
1.03	1.30	1.34	1.95	2.26	2.51	3.24	2.98
Rb	Sr	In	Sn	Sb	Te	I	Xe
0.82	*0.95*	*1.78*	*1.96*	*2.05*	*2.10*	*2.66*	*2.6*
0.99	1.21	1.30	1.83	2.06	2.34	2.88	2.59
Cs	Ba	Tl	Pb	Bi			
0.79	*0.89*	*2.04*	*2.33*	*2.02*			

Data: Pauling values: A.L. Allred, *J. Inorg. Nucl. Chem.* 17, 215 (1961); L.C. Allen and J.E. Huheey, *ibid.*, 42, 1523 (1980). Mulliken values: L.C. Allen, *J. Am. Chem. Soc.* 111, 9003 (1989). The Mulliken values have been scaled to the range of the Pauling values.

Table 16.2 Properties of diatomic molecules

	$\tilde{\nu}_e/cm^{-1}$	θ_V/K	B/cm^{-1}	θ_R/K	r/pm	$k/(N\,m^{-1})$	$D/(kJ\,mol^{-1})$	σ
$^1H_2^+$	2321.8	3341	29.8	42.9	106	160	255.8	2
$^1H_2$	4400.39	6332	60.864	87.6	74.138	574.9	432.1	2
$^2H_2$	3118.46	4487	30.442	43.8	74.154	577.0	439.6	2
$^1H^{19}F$	4138.32	5955	20.956	30.2	91.680	965.7	564.4	1
$^1H^{35}Cl$	2990.95	4304	10.593	15.2	127.45	516.3	427.7	1
$^1H^{81}Br$	2648.98	3812	8.465	12.2	141.44	411.5	362.7	1
$^1H^{127}I$	2308.09	3321	6.511	9.37	160.92	313.8	294.9	1
$^{14}N_2$	2358.07	3393	1.9987	2.88	109.76	2293.8	941.7	2
$^{16}O_2$	1580.36	2274	1.4457	2.08	120.75	1176.8	493.5	2
$^{19}F_2$	891.8	1283	0.8828	1.27	141.78	445.1	154.4	2
$^{35}Cl_2$	559.71	805	0.2441	0.351	198.75	322.7	239.3	2
$^{12}C^{16}O$	2170.21	3122	1.9313	2.78	112.81	1903.17	1071.8	1
$^{79}Br^{81}Br$	323.2	465	0.0809	10.116	283.3	245.9	190.2	1

Data: AIP

Table 16.3 Typical vibrational wavenumbers, $\tilde{\nu}/cm^{-1}$

C—H stretch	2850–2960	C—F stretch	1000–1400
C—H bend	1340–1465	C—Cl stretch	600–800
C—C stretch, bend	700–1250	C—Br stretch	500–600
C=C stretch	1620–1680	C—I stretch	500
C≡C stretch	2100–2260	CO_3^{2-}	1410–1450
O—H stretch	3590–3650	NO_3^-	1350–1420
H-bonds	3200–3570	NO_2^-	1230–1250
C=O stretch	1640–1780	SO_4^{2-}	1080–1130
C≡N stretch	2215–2275	Silicates	900–1100
N—H stretch	3200–3500		

Data: L.J. Bellamy, *The infrared spectra of complex molecules* and *Advances in infrared group frequencies*. Chapman and Hall.

Table 17.1 Colour, frequency, and energy of light

Colour	λ/nm	$\nu/(10^{14}\,Hz)$	$\tilde{\nu}/(10^4\,cm^{-1})$	E/eV	$E/(kJ\,mol^{-1})$
Infrared	> 1000	< 3.00	< 1.00	< 1.24	< 120
Red	700	4.28	1.43	1.77	171
Orange	620	4.84	1.61	2.00	193
Yellow	580	5.17	1.72	2.14	206
Green	530	5.66	1.89	2.34	226
Blue	470	6.38	2.13	2.64	254
Violet	420	7.14	2.38	2.95	285
Near ultraviolet	300	10.0	3.33	4.15	400
Far ultraviolet	< 200	> 15.0	> 5.00	> 6.20	> 598

Data: J.G. Calvert and J.N. Pitts, *Photochemistry*. Wiley, New York (1966).

Table 17.2 Absorption characteristics of some groups and molecules

Group	$\tilde{\nu}_{max}/(10^4\ cm^{-1})$	λ_{max}/nm	$\varepsilon_{max}/(L\ mol^{-1}\ cm^{-1})$
C=C($\pi^* \leftarrow \pi$)	6.10	163	1.5×10^4
	5.73	174	5.5×10^3
C=O($\pi^* \leftarrow$ n)	3.7–3.5	270–290	10–20
—N=N—	2.9	350	15
	> 3.9	< 260	Strong
$—NO_2$	3.6	280	10
	4.8	210	1.0×10^4
$C_6H_5—$	3.9	255	200
	5.0	200	6.3×10^3
	5.5	180	1.0×10^5
$[Cu(OH_2)_6]^{2+}$(aq)	1.2	810	10
$[Cu(NH_3)_4]^{2+}$(aq)	1.7	600	50
$H_2O(\pi^* \leftarrow n)$	6.0	167	7.0×10^3

Table 18.1 Nuclear spin properties

Nuclide	Natural abundance %	Spin I	Magnetic moment μ/μ_N	g-value	$\gamma/(10^7\ T^{-1}\ s^{-1})$	NMR frequency at 1 T, ν/MHz
$^1n^*$		$\frac{1}{2}$	−1.9130	−3.8260	−18.324	29.167
^1H	99.9844	$\frac{1}{2}$	2.792 85	5.5857	26.752	42.576
^2H	0.0156	1	0.857 45	0.857 45	4.1067	6.536
$^3H^*$		$\frac{1}{2}$	−2.127 65	−4.2553	−20.380	32.434
^{10}B	19.6	3	1.8005	0.6002	2.875	4.574
^{11}B	80.4	$\frac{3}{2}$	2.6884	1.7923	8.5841	13.660
^{13}C	1.108	$\frac{1}{2}$	0.7023	1.4046	6.7272	10.705
^{14}N	99.635	1	0.403 56	0.403 56	1.9328	3.076
^{17}O	0.037	$\frac{5}{2}$	−1.893	−0.7572	−3.627	5.772
^{19}F	100	$\frac{1}{2}$	2.628 35	5.2567	25.177	40.054
^{31}P	100	$\frac{1}{2}$	1.1317	2.2634	10.840	17.238
^{33}S	0.74	$\frac{3}{2}$	0.6434	0.4289	2.054	3.266
^{35}Cl	75.4	$\frac{3}{2}$	0.8218	0.5479	2.624	4.171
^{37}Cl	24.6	$\frac{3}{2}$	0.6841	0.4561	2.184	3.472

* Radioactive.

μ is the magnetic moment of the spin state with the largest value of m_I: $\mu = g_I \mu_N I$ and μ_N is the nuclear magneton (see inside front cover).

Data: KL

Table 18.2 Hyperfine coupling constants for atoms, a/mT

Nuclide	Spin	Isotropic coupling	Anisotropic coupling
^{1}H	$\frac{1}{2}$	50.8(1*s*)	
^{2}H	1	7.8(1*s*)	
^{13}C	$\frac{1}{2}$	113.0(2*s*)	6.6(2*p*)
^{14}N	1	55.2(2*s*)	4.8(2*p*)
^{19}F	$\frac{1}{2}$	1720(2*s*)	108.4(2*p*)
^{31}P	$\frac{1}{2}$	364(3*s*)	20.6(3*p*)
^{35}Cl	$\frac{3}{2}$	168(3*s*)	10.0(3*p*)
^{37}Cl	$\frac{3}{2}$	140(3*s*)	8.4(3*p*)

Data: P.W. Atkins and M.C.R. Symons, *The structure of inorganic radicals*. Elsevier, Amsterdam (1967).

Table 21.3 Ionic radii (r/pm)†

Li^{+}(4)	Be^{2+}(4)	B^{3+}(4)	N^{3-}	O^{2-}(6)	F^{-}(6)
59	27	12	171	140	133
Na^{+}(6)	Mg^{2+}(6)	Al^{3+}(6)	P^{3-}	S^{2-}(6)	Cl^{-}(6)
102	72	53	212	184	181
K^{+}(6)	Ca^{2+}(6)	Ga^{3+}(6)	As^{3-}(6)	Se^{2-}(6)	Br^{-}(6)
138	100	62	222	198	196
Rb^{+}(6)	Sr^{2+}(6)	In^{3+}(6)		Te^{2-}(6)	I^{-}(6)
149	116	79		221	220
Cs^{+}(6)	Ba^{2+}(6)	Tl^{3+}(6)			
167	136	88			

d-block elements (high-spin ions)

Sc^{3+}(6)	Ti^{4+}(6)	Cr^{3+}(6)	Mn^{3+}(6)	Fe^{2+}(6)	Co^{3+}(6)	Cu^{2+}(6)	Zn^{2+}(6)
73	60	61	65	63	61	73	75

† Numbers in parentheses are the coordination numbers of the ions. Values for ions without a coordination number stated are estimates.
Data: R.D. Shannon and C.T. Prewitt, *Acta Cryst.* B25, 925 (1969).

Table 22.1 Dipole moments, polarizabilities, and polarizability volumes

	$\mu/(10^{-30}\ \mathrm{C\,m})$	μ/D	$\alpha'/(10^{-30}\ \mathrm{m}^3)$	$\alpha'/(10^{-40}\ \mathrm{J^{-1}\,C^2\,m^2})$
Ar	0	0	1.66	1.85
C_2H_5OH	5.64	1.69		
$C_6H_5CH_3$	1.20	0.36		
C_6H_6	0	0	10.4	11.6
CCl_4	0	0	10.5	11.7
CH_2Cl_2	5.24	1.57	6.80	7.57
CH_3Cl	6.24	1.87	4.53	5.04
CH_3OH	5.70	1.71	3.23	3.59
CH_4	0	0	2.60	2.89
$CHCl_3$	3.37	1.01	8.50	9.46
CO	0.390	0.117	1.98	2.20
CO_2	0	0	2.63	2.93
H_2	0	0	0.819	0.911
H_2O	6.17	1.85	1.48	1.65
HBr	2.67	0.80	3.61	4.01
HCl	3.60	1.08	2.63	2.93
He	0	0	0.20	0.22
HF	6.37	1.91	0.51	0.57
HI	1.40	0.42	5.45	6.06
N_2	0	0	1.77	1.97
NH_3	4.90	1.47	2.22	2.47
$1,2\text{-}C_6H_4(CH_3)_2$	2.07	0.62		

Data: HCP and C.J.F. Böttcher and P. Bordewijk, *Theory of electric polarization*. Elsevier, Amsterdam (1978).

Table 22.2 Refractive indices relative to air at 20°C

	434 nm	589 nm	656 nm
Benzene	1.5236	1.5012	1.4965
Carbon tetrachloride	1.4729	1.4676	1.4579
Carbon disulfide	1.6748	1.6276	1.6182
Ethanol	1.3700	1.3618	1.3605
KCl(s)	1.5050	1.4904	1.4973
KI(s)	1.7035	1.6664	1.6581
Methanol	1.3362	1.3290	1.3277
Methylbenzene	1.5170	1.4955	1.4911
Water	1.3404	1.3330	1.3312

Data: AIP

Table 22.4 Lennard-Jones (12,6)-potential parameters

	(ε/k)/K	r_0/pm
Ar	111.84	362.3
C_2H_2	209.11	463.5
C_2H_4	200.78	458.9
C_2H_6	216.12	478.2
C_6H_6	377.46	617.4
CCl_4	378.86	624.1
Cl_2	296.27	448.5
CO_2	201.71	444.4
F_2	104.29	357.1
Kr	154.87	389.5
N_2	91.85	391.9
O_2	113.27	365.4
Xe	213.96	426.0

Source: F. Cuadros, I. Cachadiña, and W. Ahamuda, *Molec. Engineering*, 6, 319 (1996).

Table 22.5 Magnetic susceptibilities at 298 K

	$\chi/10^{-6}$	$\chi_m/(10^{-4}\ \mathrm{cm^3\ mol^{-1}})$
Water	−90	−16.0
Benzene	−7.2	−6.4
Cyclohexane	−7.9	−8.5
Carbon tetrachloride	−8.9	−8.4
NaCl(s)	−13.9	−3.75
Cu(s)	−96	−6.8
S(s)	−12.9	−2.0
Hg(l)	−28.5	−4.2
$CuSO_4{\cdot}5H_2O$(s)	+176	+192
$MnSO_4{\cdot}4H_2O$(s)	+2640	$+2.79 \times 10^3$
$NiSO_4{\cdot}7H_2O$(s)	+416	+600
$FeSO_4(NH_4)_2SO_4{\cdot}6H_2O$(s)	+755	$+1.51 \times 10^3$
Al(s)	+22	+2.2
Pt(s)	+262	+22.8
Na(s)	+7.3	+1.7
K(s)	+5.6	+2.5

Data: KL and $\chi_m = \chi M/\rho$.

Table 23.1 Frictional coefficients and molecular geometry

Major axis/ Minor axis	Prolate	Oblate
2	1.04	1.04
3	1.11	1.10
4	1.18	1.17
5	1.25	1.22
6	1.31	1.28
7	1.38	1.33
8	1.43	1.37
9	1.49	1.42
10	1.54	1.46
50	2.95	2.38
100	4.07	2.97

Data: K.E. Van Holde, *Physical biochemistry*. Prentice-Hall, Englewood Cliffs (1971).

Sphere; radius a, $c = a$ f_0

Prolate ellipsoid; major axis $2a$, minor axis $2b$, $c = (ab^2)^{1/3}$

$$\left\{\frac{(1-b^2/a^2)^{1/2}}{(b/a)^{2/3}\ \ln\{[1+(1-b^2/a^2)^{1/2}]/(b/a)\}}\right\}f_0$$

Oblate ellipsoid; major axis $2a$, minor axis $2b$, $c = (a^2b)^{1/3}$

$$\left\{\frac{(a^2/b^2-1)^{1/2}}{(a/b)^{2/3}\ \arctan\,[(a^2/b^2-1)^{1/2}]}\right\}f_0$$

Long rod; length l, radius a, $c = (3a^2/4)^{1/3}$

$$\left\{\frac{(l/2a)^{2/3}}{(3/2)^{1/3}\{2\ \ln\,(l/a)-0.11\}}\right\}f_0$$

In each case $f_0 = 6\pi\eta c$ with the appropriate value of c.

Table 23.2 Diffusion coefficients of macromolecules in water at 20°C

	$M/(\mathrm{kg\ mol^{-1}})$	$D/(10^{-10}\ \mathrm{m^2\ s^{-1}})$
Sucrose	0.342	4.586
Ribonuclease	13.7	1.19
Lysozyme	14.1	1.04
Serum albumin	65	0.594
Haemoglobin	68	0.69
Urease	480	0.346
Collagen	345	0.069
Myosin	493	0.116

Data: C. Tanford, *Physical chemistry of macromolecules*. Wiley, New York (1961).

Table 23.3 Intrinsic viscosity

Macromolecule	Solvent	$\theta/^{\circ}C$	$K/(10^{-3}\ cm^3\ g^{-1})$	a
Polystyrene	Benzene	25	9.5	0.74
	Cyclohexane	34†	81	0.50
Polyisobutylene	Benzene	23†	83	0.50
	Cyclohexane	30	26	0.70
Amylose	0.33 M KCl(aq)	25†	113	0.50
Various protein‡	Guanidine hydrochloride + $HSCH_2CH_2OH$		7.16	0.66

† The θ temperature.
‡ Use $[\eta]=KN^a$; N is the number of amino acid residues.
Data: K.E. Van Holde, *Physical biochemistry*. Prentice-Hall, Englewood Cliffs (1971).

Table 23.4 Radius of gyration of some macromolecules

	$M/(kg\ mol^{-1})$	R_g/nm
Serum albumin	66	2.98
Myosin	493	46.8
Polystyrene	3.2×10^3	50 (in poor solvent)
DNA	4×10^3	117.0
Tobacco mosaic virus	3.9×10^4	92.4

Data: C. Tanford, *Physical chemistry of macromolecules*. Wiley, New York (1961).

Table 24.1 Transport properties of gases at 1 atm

	$\kappa/(J\ K^{-1}\ m^{-1}\ s^{-1})$	$\eta/\mu P$	
	273 K	273 K	293 K
Air	0.0241	173	182
Ar	0.0163	210	223
C_2H_4	0.0164	97	103
CH_4	0.0302	103	110
Cl_2	0.079	123	132
CO_2	0.0145	136	147
H_2	0.1682	84	88
He	0.1442	187	196
Kr	0.0087	234	250
N_2	0.0240	166	176
Ne	0.0465	298	313
O_2	0.0245	195	204
Xe	0.0052	212	228

Data: KL

Table 24.3 Viscosities of liquids at 298 K, $\eta/(10^{-3}\ kg\ m^{-1}\ s^{-1})$

Benzene	0.601
Carbon tetrachloride	0.880
Ethanol	1.06
Mercury	1.55
Methanol	0.553
Pentane	0.224
Sulfuric acid	27
Water†	0.891

† The viscosity of water over its entire liquid range is represented with less than 1 per cent error by the expression

$$\log(\eta_{20}/\eta) = A/B,$$

$$A = 1.37023(t-20) + 8.36 \times 10^{-4}\,(t-20)^2$$

$$B = 109 + t \qquad t = \theta/^{\circ}C$$

Convert $kg\,m^{-1}s^{-1}$ to centipoise (cP) by multiplying by 10^3 (so $\eta \approx 1$ cP for water).
Data: AIP, KL

Table 24.4 Limiting ionic conductivities in water at 298 K, $\lambda/(\text{mS m}^2\ \text{mol}^{-1})$

Cations		Anions	
Ba^{2+}	12.72	Br^-	7.81
Ca^{2+}	11.90	$CH_3CO_2^-$	4.09
Cs^+	7.72	Cl^-	7.635
Cu^{2+}	10.72	ClO_4^-	6.73
H^+	34.96	CO_3^{2-}	13.86
K^+	7.350	$(CO_2)_2^{2-}$	14.82
Li^+	3.87	F^-	5.54
Mg^{2+}	10.60	$[Fe(CN)_6]^{3-}$	30.27
Na^+	5.010	$[Fe(CN)_6]^{4-}$	44.20
$[N(C_2H_5)_4]^+$	3.26	HCO_2^-	5.46
$[N(CH_3)_4]^+$	4.49	I^-	7.68
NH_4^+	7.35	NO_3^-	7.146
Rb^+	7.78	OH^-	19.91
Sr^{2+}	11.89	SO_4^{2-}	16.00
Zn^{2+}	10.56		

Data: KL, RS

Table 24.5 Ionic mobilities in water at 298 K, $u/(10^{-8}\ \text{m}^2\ \text{s}^{-1}\ \text{V}^{-1})$

Cations		Anions	
Ag^+	6.42	Br^-	8.09
Ca^{2+}	6.17	$CH_3CO_2^-$	4.24
Cu^{2+}	5.56	Cl^-	7.91
H^+	36.23	CO_3^{2-}	7.46
K^+	7.62	F^-	5.70
Li^+	4.01	$[Fe(CN)_6]^{3-}$	10.5
Na^+	5.19	$[Fe(CN)_6]^{4-}$	11.4
NH_4^+	7.63	I^-	7.96
$[N(CH_3)_4]^+$	4.65	NO_3^-	7.40
Rb^+	7.92	OH^-	20.64
Zn^{2+}	5.47	SO_4^{2-}	8.29

Data: Principally Table 24.4 and $u = \lambda/zF$

Table 24.6 Debye–Hückel–Onsager coefficients for (1,1)-electrolytes at 25 °C

Solvent	$A/(\text{mS m}^2\ \text{mol}^{-1}/(\text{mol L}^{-1})^{1/2})$	$B/(\text{mol L}^{-1})^{-1/2}$
Acetone (propanone)	3.28	1.63
Acetonitrile	2.29	0.716
Ethanol	8.97	1.83
Methanol	15.61	0.923
Nitrobenzene	4.42	0.776
Nitromethane	111	0.708
Water	60.20	0.229

Data: J.O'M. Bockris and A.K.N. Reddy, *Modern electrochemistry*. Plenum, New York (1970).

Table 24.7 Diffusion coefficients at 25 °C, $D/(10^{-9}\ \text{m}^2\ \text{s}^{-1})$

Molecules in liquids				Ions in water			
I_2 in hexane	4.05	H_2 in CCl_4(l)	9.75	K^+	1.96	Br^-	2.08
in benzene	2.13	N_2 in CCl_4(l)	3.42	H^+	9.31	Cl^-	2.03
CCl_4 in heptane	3.17	O_2 in CCl_4(l)	3.82	Li^+	1.03	F^-	1.46
Glycine in water	1.055	Ar in CCl_4(l)	3.63	Na^+	1.33	I^-	2.05
Dextrose in water	0.673	CH_4 in CCl_4(l)	2.89			OH^-	5.30
Sucrose in water	0.5216	H_2O in water	2.26				
		CH_3OH in water	1.58				
		C_2H_5OH in water	1.24				

Data: AIP and (for the ions) $\lambda = zuF$ in conjunction with Table 24.5.

able 25.1 Kinetic data for first-order reactions

	Phase	θ/°C	k/s^{-1}	$t_{1/2}$
$N_2O_5 \rightarrow 4NO_2 + O_2$	g	25	3.38×10^{-5}	5.70 h
	HNO_3(l)	25	1.47×10^{-6}	131 h
	Br_2(l)	25	4.27×10^{-5}	4.51 h
$C_2H_6 \rightarrow 2CH_3$	g	700	5.36×10^{-4}	21.6 min
Cyclopropane → propene	g	500	6.71×10^{-4}	17.2 min
$CH_3N_2CH_3 \rightarrow C_2H_6 + N_2$	g	327	3.4×10^{-4}	34 min
Sucrose → glucose + fructose	aq(H^+)	25	6.0×10^{-5}	3.2 h

): High pressure gas-phase limit.
Data: Principally K.J. Laidler, *Chemical kinetics*. Harper & Row, New York (1987); M.J. Pilling and P.W. Seakins, *Reaction kinetics*. Oxford University Press (1995); J. Nicholas, *Chemical kinetics*. Harper & Row, New York (1976). See also JL.

Table 25.2 Kinetic data for second-order reactions

	Phase	θ/°C	k/(L mol^{-1} s^{-1})
$2NOBr \rightarrow 2NO + Br_2$	g	10	0.80
$2NO_2 \rightarrow 2NO + O_2$	g	300	0.54
$H_2 + I_2 \rightarrow 2HI$	g	400	2.42×10^{-2}
$D_2 + HCl \rightarrow DH + DCl$	g	600	0.141
$2I \rightarrow I_2$	g	23	7×10^{9}
	hexane	50	1.8×10^{10}
$CH_3Cl + CH_3O^-$	methanol	20	2.29×10^{-6}
$CH_3Br + CH_3O^-$	methanol	20	9.23×10^{-6}
$H^+ + OH^- \rightarrow H_2O$	water	25	1.35×10^{11}
	ice	−10	8.6×10^{12}

Data: Principally K.J. Laidler, *Chemical kinetics*. Harper & Row, New York (1987); M.J. Pilling and P.W. Seakins, *Reaction kinetics*. Oxford University Press (1995); J. Nicholas, *Chemical kinetics*. Harper & Row, New York (1976).

Table 25.4 Arrhenius parameters

First-order reactions	A/s^{-1}	E_a/(kJ mol^{-1})
Cyclopropane → propene	1.58×10^{15}	272
$CH_3NC \rightarrow CH_3CN$	3.98×10^{13}	160
cis-CHD=CHD → *trans*-CHD=CHD	3.16×10^{12}	256
Cyclobutane → $2C_2H_4$	3.98×10^{15}	261
$C_2H_5I \rightarrow C_2H_4 + HI$	2.51×10^{13}	209
$C_2H_6 \rightarrow 2CH_3$	2.51×10^{17}	384
$2N_2O_5 \rightarrow 4NO_2 + O_2$	4.94×10^{13}	103
$N_2O \rightarrow N_2 + O$	7.94×10^{11}	250
$C_2H_5 \rightarrow C_2H_4 + H$	1.0×10^{13}	167
Second-order, gas-phase	A/(L mol^{-1} s^{-1})	E_a/(kJ mol^{-1})
$O + N_2 \rightarrow NO + N$	1×10^{11}	315
$OH + H_2 \rightarrow H_2O + H$	8×10^{10}	42
$Cl + H_2 \rightarrow HCl + H$	8×10^{10}	23
$2CH_3 \rightarrow C_2H_6$	2×10^{10}	ca. 0
$NO + Cl_2 \rightarrow NOCl + Cl$	4.0×10^{9}	85
$SO + O_2 \rightarrow SO_2 + O$	3×10^{8}	27
$CH_3 + C_2H_6 \rightarrow CH_4 + C_2H_5$	2×10^{8}	44
$C_6H_5 + H_2 \rightarrow C_6H_6 + H$	1×10^{8}	ca. 25
Second-order, solution	A/(L mol^{-1} s^{-1})	E_a/(kJ mol^{-1})
$C_2H_5ONa + CH_3I$ in ethanol	2.42×10^{11}	81.6
$C_2H_5Br + OH^-$ in water	4.30×10^{11}	89.5
$C_2H_5I + C_2H_5O^-$ in ethanol	1.49×10^{11}	86.6
$CH_3I + C_2H_5O^-$ in ethanol	2.42×10^{11}	81.6
$C_2H_5Br + OH^-$ in ethanol	4.30×10^{11}	89.5
$CO_2 + OH^-$ in water	1.5×10^{10}	38
$CH_3I + S_2O_3^{2-}$ in water	2.19×10^{12}	78.7
Sucrose + H_2O in acidic water	1.50×10^{15}	107.9
$(CH_3)_3CCl$ solvolysis		
in water	7.1×10^{16}	100
in methanol	2.3×10^{13}	107
in ethanol	3.0×10^{13}	112
in acetic acid	4.3×10^{13}	111
in chloroform	1.4×10^{4}	45
$C_6H_5NH_2 + C_6H_5COCH_2Br$		
in benzene	91	34

Data: Principally J. Nicholas, *Chemical kinetics*. Harper & Row, New York (1976) and A.A. Frost and R.G. Pearson, *Kinetics and mechanism*. Wiley, New York (1961).

Table 27.1 Arrhenius parameters for gas-phase reactions

	$A/(\text{L mol}^{-1}\text{s}^{-1})$			
	Experiment	Theory	$E_a/(\text{kJ mol}^{-1})$	P
$2NOCl \rightarrow 2NO + Cl_2$	9.4×10^9	5.9×10^{10}	102.0	0.16
$2NO_2 \rightarrow 2NO + O_2$	2.0×10^9	4.0×10^{10}	111.0	5.0×10^{-2}
$2ClO \rightarrow Cl_2 + O_2$	6.3×10^7	2.5×10^{10}	0.0	2.5×10^{-3}
$H_2 + C_2H_4 \rightarrow C_2H_6$	1.24×10^6	7.3×10^{11}	180	1.7×10^{-6}
$K + Br_2 \rightarrow KBr + Br$	1.0×10^{12}	2.1×10^{11}	0.0	4.8

Data: Principally M.J. Pilling and P.W. Seakins, *Reaction kinetics*. Oxford University Press (1995).

Table 27.2 Arrhenius parameters for reactions in solution. See Table 25.4

Table 28.1 Maximum observed enthalpies of physisorption, $\Delta_{ad}H^{\ominus}/(\text{kJ mol}^{-1})$

C_2H_2	−38
C_2H_4	−34
CH_4	−21
Cl_2	−36
CO	−25
CO_2	−25
H_2	−84
H_2O	−59
N_2	−21
NH_3	−38
O_2	−21

Data: D.O. Haywood and B.M.W. Trapnell, *Chemisorption*. Butterworth (1964).

Table 28.2 Enthalpies of chemisorption, $\Delta_{ad}H^{\ominus}/(\text{kJ mol}^{-1})$

	Adsorbent (substrate)											
Adsorbate	Ti	Ta	Nb	W	Cr	Mo	Mn	Fe	Co	Ni	Rh	Pt
H_2		−188			−188	−167	−71	−134			−117	
N_2		−586						−293				
O_2						−720					−494	−293
CO	−640							−192	−176			
CO_2	−682	−703	−552	−456	−339	−372	−222	−225	−146	−184		
NH_3				−301				−188		−155		
C_2H_4		−577		−427	−427			−285		−243	−209	

Data: D.O. Haywood and B.M.W. Trapnell, *Chemisorption*. Butterworth (1964).

Table 28.3 Activation energies of catalysed reactions

	Catalyst	$E_a/(\text{kJ mol}^{-1})$
$2HI \rightarrow H_2 + I_2$	None	184
	Au(s)	105
	Pt(s)	59
$2NH_3 \rightarrow N_2 + 3H_2$	None	350
	W(s)	162
$2N_2O \rightarrow 2N_2 + O_2$	None	245
	Au(s)	121
	Pt(s)	134
$(C_2H_5)_2O$ pyrolysis	None	224
	I_2(g)	144

Data: G.C. Bond, *Heterogeneous catalysis*. Clarendon Press, Oxford (1986).

Table 29.1 Exchange current densities and transfer coefficients at 298 K

Reaction	Electrode	$j_0/(\text{A cm}^{-2})$	α
$2H^+ + 2e^- \rightarrow H_2$	Pt	7.9×10^{-4}	
	Cu	1×10^{-6}	
	Ni	6.3×10^{-6}	0.58
	Hg	7.9×10^{-13}	0.50
	Pb	5.0×10^{-12}	
$Fe^{3+} + e^- \rightarrow Fe^{2+}$	Pt	2.5×10^{-3}	0.58
$Ce^{4+} + e^- \rightarrow Ce^{3+}$	Pt	4.0×10^{-5}	0.75

Data: Principally J.O'M. Bockris and A.K.N. Reddy, *Modern electrochemistry*. Plenum, New York (1970).

Character tables

The groups C_1, C_s, C_i

C_1 (1)	E	$h = 1$
A	1	

$C_s = C_h$ (*m*)	E	σ_h	$h = 2$	
A′	1	1	x, y, R_z	x^2, y^2, z^2, xy
A″	1	−1	z, R_x, R_y	yz, xz

$C_i = S_2$ (1)	E	i	$h = 2$	
A_g	1	1	R_x, R_y, R_z	$x^2, y^2, z^2, xy, xz, yz$
A_u	1	−1	x, y, z	

The groups C_{nv}

C_{2v}, 2*mm*	E	C_2	σ_v	σ_v'	$h = 4$	
A_1	1	1	1	1	z, z^2, x^2, y^2	
A_2	1	1	−1	−1	xy	R_z
B_1	1	−1	1	−1	x, xz	R_y
B_2	1	−1	−1	1	y, yz	R_x

C_{3v}, 3*m*	E	$2C_3$	$3\sigma_v$	$h = 6$	
A_1	1	1	1	$z, z^2, x^2 + y^2$	
A_2	1	1	−1		R_z
E	2	−1	0	$(x, y), (xy, x^2 - y^2)(xz, yz)$	(R_x, R_y)

C_{4v}, 4*mm*	E	C_2	$2C_4$	$2\sigma_v$	$2\sigma_d$	$h = 8$	
A_1	1	1	1	1	1	$z, z^2, x^2 + y^2$	
A_2	1	1	1	−1	−1		R_z
B_1	1	1	−1	1	−1	$x^2 - y^2$	
B_2	1	1	−1	−1	1	xy	
E	2	−2	0	0	0	$(x, y), (xz, yz)$	(R_x, R_y)

The icosahedral group

I	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	$h = 60$	
A	1	1	1	1	1		$z^2 + y^2 + z^2$
T_1	3	$\frac{1}{2}(1+\sqrt{5})$	$\frac{1}{2}(1-\sqrt{5})$	0	-1	(x, y, z) (R_x, R_y, R_z)	
T_2	3	$\frac{1}{2}(1-\sqrt{5})$	$\frac{1}{2}(1+\sqrt{5})$	0	-1		
G	4	-1	-1	1	0		
G	5	0	0	-1	1		$(2z^2 - x^2 - y^2, x^2 - y^2, xy, yz, zx)$

Further information: P.W. Atkins, M.S. Child, and C.S.G. Phillips, *Tables for group theory*. Oxford University Press (1970).