

Data section

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1 Important values, constants and standards

molar gas constant	$R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$
Faraday constant	$F = 9.65 \times 10^4 \text{ C mol}^{-1}$
Avogadro constant	$L = 6.022 \times 10^{23} \text{ mol}^{-1}$
electronic charge	$e = -1.60 \times 10^{-19} \text{ C}$
molar volume of gas	$V_m = 22.4 \text{ dm}^3 \text{ mol}^{-1}$ at s.t.p. (101 kPa and 273 K) $V_m = 24.0 \text{ dm}^3 \text{ mol}^{-1}$ at room conditions
ionic product of water	$K_w = 1.00 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$ (at 298 K (25 °C))
specific heat capacity of water	$c = 4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$ ($4.18 \text{ J g}^{-1} \text{ K}^{-1}$)

2 Ionisation energies (1st, 2nd, 3rd and 4th) of selected elements in kJ mol^{-1}

	proton number	1st	2nd	3rd	4th
H	1	1310			
He	2	2370	5250		
Li	3	519	7300	11800	
Be	4	900	1760	14800	21000
B	5	799	2420	3660	25000
C	6	1090	2350	4610	6220
N	7	1400	2860	4590	7480
O	8	1310	3390	5320	7450
F	9	1680	3370	6040	8410
Ne	10	2080	3950	6150	9290
Na	11	494	4560	6940	9540
Mg	12	736	1450	7740	10500
Al	13	577	1820	2740	11600
Si	14	786	1580	3230	4360
P	15	1060	1900	2920	4960
S	16	1000	2260	3390	4540
Cl	17	1260	2300	3850	5150
Ar	18	1520	2660	3950	5770
K	19	418	3070	4600	5860
Ca	20	590	1150	4940	6480
Sc	21	632	1240	2390	7110
Ti	22	661	1310	2720	4170
V	23	648	1370	2870	4600
Cr	24	653	1590	2990	4770
Mn	25	716	1510	3250	5190
Fe	26	762	1560	2960	5400
Co	27	757	1640	3230	5100

	proton number	1st	2nd	3rd	4th
Ni	28	736	1750	3390	5400
Cu	29	745	1960	3350	5690
Zn	30	908	1730	3828	5980
Ga	31	577	1980	2960	6190
Br	35	1140	2080	3460	4850
Rb	37	403	2632	3900	5080
Sr	38	548	1060	4120	5440
Ag	47	731	2074	3361	5000
I	53	1010	1840	3000	4030
Cs	55	376	2420	3300	4400
Ba	56	502	966	3390	4700

3 Bond energies

3(a) Bond energies in diatomic molecules (these are exact values)

Homonuclear

bond	energy / kJ mol⁻¹
H–H	436
N≡N	944
O=O	496
P≡P	485
S=S	425
F–F	158
Cl–Cl	242
Br–Br	193
I–I	151

Heteronuclear

bond	energy / kJ mol⁻¹
H–F	562
H–Cl	431
H–Br	366
H–I	299
C≡O	1077

3(b) Bond energies in polyatomic molecules (these are average values)

Homonuclear

bond	energy/kJ mol ⁻¹
C–C	350
C=C	610
C≡C	840
C $\equiv$ C (benzene)	520
N–N	160
N=N	410
O–O	150
Si–Si	225
P–P	200
S–S	265

Heteronuclear

bond	energy/kJ mol ⁻¹
C–H	410
C–Cl	340
C–Br	280
C–I	240
C–N	305
C=N	610
C≡N	890
C–O	360
C=O	740
C=O in CO ₂	805
N–H	390
N–Cl	310
O–H	460
Si–Cl	360
Si–H	320
Si–O (in SiO ₂ (s))	460
Si=O (in SiO ₂ (g))	640
P–H	320
P–Cl	330
P–O	340
P=O	540
S–H	340
S–Cl	250
S–O	360
S=O	500

4 Standard electrode (reduction) potentials, $E^\ominus$, at 298 K (25 °C) $E^\ominus$ in alphabetical order

electrode reaction	$E^\ominus / \text{V}$
$\text{Ag}^+ + \text{e}^- \rightleftharpoons \text{Ag}$	+0.80
$\text{Al}^{3+} + 3\text{e}^- \rightleftharpoons \text{Al}$	-1.66
$\text{Ba}^{2+} + 2\text{e}^- \rightleftharpoons \text{Ba}$	-2.90
$\text{Br}_2 + 2\text{e}^- \rightleftharpoons 2\text{Br}^-$	+1.07
$\text{Ca}^{2+} + 2\text{e}^- \rightleftharpoons \text{Ca}$	-2.87
$\text{Cl}_2 + 2\text{e}^- \rightleftharpoons 2\text{Cl}^-$	+1.36
$2\text{HOCl} + 2\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{Cl}_2 + 2\text{H}_2\text{O}$	+1.64
$\text{ClO}^- + \text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons \text{Cl}^- + 2\text{OH}^-$	+0.89
$\text{Co}^{2+} + 2\text{e}^- \rightleftharpoons \text{Co}$	-0.28
$\text{Co}^{3+} + \text{e}^- \rightleftharpoons \text{Co}^{2+}$	+1.82
$[\text{Co}(\text{NH}_3)_6]^{2+} + 2\text{e}^- \rightleftharpoons \text{Co} + 6\text{NH}_3$	-0.43
$\text{Cr}^{2+} + 2\text{e}^- \rightleftharpoons \text{Cr}$	-0.91
$\text{Cr}^{3+} + 3\text{e}^- \rightleftharpoons \text{Cr}$	-0.74
$\text{Cr}^{3+} + \text{e}^- \rightleftharpoons \text{Cr}^{2+}$	-0.41
$\text{Cr}_2\text{O}_7^{2-} + 14\text{H}^+ + 6\text{e}^- \rightleftharpoons 2\text{Cr}^{3+} + 7\text{H}_2\text{O}$	+1.33
$\text{Cu}^+ + \text{e}^- \rightleftharpoons \text{Cu}$	+0.52
$\text{Cu}^{2+} + 2\text{e}^- \rightleftharpoons \text{Cu}$	+0.34
$\text{Cu}^{2+} + \text{e}^- \rightleftharpoons \text{Cu}^+$	+0.15
$[\text{Cu}(\text{NH}_3)_4]^{2+} + 2\text{e}^- \rightleftharpoons \text{Cu} + 4\text{NH}_3$	-0.05
$\text{F}_2 + 2\text{e}^- \rightleftharpoons 2\text{F}^-$	+2.87
$\text{Fe}^{2+} + 2\text{e}^- \rightleftharpoons \text{Fe}$	-0.44
$\text{Fe}^{3+} + 3\text{e}^- \rightleftharpoons \text{Fe}$	-0.04
$\text{Fe}^{3+} + \text{e}^- \rightleftharpoons \text{Fe}^{2+}$	+0.77
$[\text{Fe}(\text{CN})_6]^{3-} + \text{e}^- \rightleftharpoons [\text{Fe}(\text{CN})_6]^{4-}$	+0.36
$\text{Fe}(\text{OH})_3 + \text{e}^- \rightleftharpoons \text{Fe}(\text{OH})_2 + \text{OH}^-$	-0.56
$2\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{H}_2$	0.00

electrode reaction	$E^{\ominus} / \text{V}$
$2\text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons \text{H}_2 + 2\text{OH}^-$	-0.83
$\text{I}_2 + 2\text{e}^- \rightleftharpoons 2\text{I}^-$	+0.54
$\text{K}^+ + \text{e}^- \rightleftharpoons \text{K}$	-2.92
$\text{Li}^+ + \text{e}^- \rightleftharpoons \text{Li}$	-3.04
$\text{Mg}^{2+} + 2\text{e}^- \rightleftharpoons \text{Mg}$	-2.38
$\text{Mn}^{2+} + 2\text{e}^- \rightleftharpoons \text{Mn}$	-1.18
$\text{Mn}^{3+} + \text{e}^- \rightleftharpoons \text{Mn}^{2+}$	+1.49
$\text{MnO}_2 + 4\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{Mn}^{2+} + 2\text{H}_2\text{O}$	+1.23
$\text{MnO}_4^- + \text{e}^- \rightleftharpoons \text{MnO}_4^{2-}$	+0.56
$\text{MnO}_4^- + 4\text{H}^+ + 3\text{e}^- \rightleftharpoons \text{MnO}_2 + 2\text{H}_2\text{O}$	+1.67
$\text{MnO}_4^- + 8\text{H}^+ + 5\text{e}^- \rightleftharpoons \text{Mn}^{2+} + 4\text{H}_2\text{O}$	+1.52
$\text{NO}_3^- + 2\text{H}^+ + \text{e}^- \rightleftharpoons \text{NO}_2 + \text{H}_2\text{O}$	+0.81
$\text{NO}_3^- + 3\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{HNO}_2 + \text{H}_2\text{O}$	+0.94
$\text{NO}_3^- + 10\text{H}^+ + 8\text{e}^- \rightleftharpoons \text{NH}_4^+ + 3\text{H}_2\text{O}$	+0.87
$\text{Na}^+ + \text{e}^- \rightleftharpoons \text{Na}$	-2.71
$\text{Ni}^{2+} + 2\text{e}^- \rightleftharpoons \text{Ni}$	-0.25
$[\text{Ni}(\text{NH}_3)_6]^{2+} + 2\text{e}^- \rightleftharpoons \text{Ni} + 6\text{NH}_3$	-0.51
$\text{H}_2\text{O}_2 + 2\text{H}^+ + 2\text{e}^- \rightleftharpoons 2\text{H}_2\text{O}$	+1.77
$\text{HO}_2^- + \text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons 3\text{OH}^-$	+0.88
$\text{O}_2 + 4\text{H}^+ + 4\text{e}^- \rightleftharpoons 2\text{H}_2\text{O}$	+1.23
$\text{O}_2 + 2\text{H}_2\text{O} + 4\text{e}^- \rightleftharpoons 4\text{OH}^-$	+0.40
$\text{O}_2 + 2\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{H}_2\text{O}_2$	+0.68
$\text{O}_2 + \text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons \text{HO}_2^- + \text{OH}^-$	-0.08
$\text{Pb}^{2+} + 2\text{e}^- \rightleftharpoons \text{Pb}$	-0.13
$\text{Pb}^{4+} + 2\text{e}^- \rightleftharpoons \text{Pb}^{2+}$	+1.69
$\text{PbO}_2 + 4\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{Pb}^{2+} + 2\text{H}_2\text{O}$	+1.47
$\text{SO}_4^{2-} + 4\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{SO}_2 + 2\text{H}_2\text{O}$	+0.17
$\text{S}_2\text{O}_8^{2-} + 2\text{e}^- \rightleftharpoons 2\text{SO}_4^{2-}$	+2.01

electrode reaction	$E^\ominus / \text{V}$
$\text{S}_4\text{O}_6^{2-} + 2\text{e}^- \rightleftharpoons 2\text{S}_2\text{O}_3^{2-}$	+0.09
$\text{Sn}^{2+} + 2\text{e}^- \rightleftharpoons \text{Sn}$	-0.14
$\text{Sn}^{4+} + 2\text{e}^- \rightleftharpoons \text{Sn}^{2+}$	+0.15
$\text{V}^{2+} + 2\text{e}^- \rightleftharpoons \text{V}$	-1.20
$\text{V}^{3+} + \text{e}^- \rightleftharpoons \text{V}^{2+}$	-0.26
$\text{VO}^{2+} + 2\text{H}^+ + \text{e}^- \rightleftharpoons \text{V}^{3+} + \text{H}_2\text{O}$	+0.34
$\text{VO}_2^+ + 2\text{H}^+ + \text{e}^- \rightleftharpoons \text{VO}^{2+} + \text{H}_2\text{O}$	+1.00
$\text{VO}_3^- + 4\text{H}^+ + \text{e}^- \rightleftharpoons \text{VO}^{2+} + 2\text{H}_2\text{O}$	+1.00
$\text{Zn}^{2+} + 2\text{e}^- \rightleftharpoons \text{Zn}$	-0.76

All ionic states refer to aqueous ions but other state symbols have been omitted.

5 Pauling electronegativity values

H 2.1																
Li 1.0	Be 1.6											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.3											Al 1.5	Si 1.9	P 2.2	S 2.6	Cl 3.0
K 0.8	Ca 1.0	Sc 1.4	Ti 1.5	V 1.6	Cr 1.7	Mn 1.5	Fe 1.8	Co 1.9	Ni 1.9	Cu 1.9	Zn 1.6	Ga 1.8	Ge 2.0	As 2.2	Se 2.6	Br 2.6

6 Typical proton (^1H) NMR chemical shift values (δ) relative to TMS = 0

environment of proton	example	chemical shift range δ/ppm
alkane	$-\text{CH}_3$, $-\text{CH}_2-$, $>\text{CH}-$	0.9–1.7
alkyl next to $\text{C}=\text{O}$	$\text{CH}_3-\text{C}=\text{O}$, $-\text{CH}_2-\text{C}=\text{O}$, $>\text{CH}-\text{C}=\text{O}$	2.2–3.0
alkyl next to aromatic ring	CH_3-Ar , $-\text{CH}_2-\text{Ar}$, $>\text{CH}-\text{Ar}$	2.3–3.0
alkyl next to electronegative atom	CH_3-O , $-\text{CH}_2-\text{O}$, $-\text{CH}_2-\text{Cl}$	3.2–4.0
attached to alkene	$=\text{CHR}$	4.5–6.0
attached to aromatic ring	$\text{H}-\text{Ar}$	6.0–9.0
aldehyde	$\text{H}-\text{COR}$	9.3–10.5
alcohol	ROH	0.5–6.0
phenol	$\text{Ar}-\text{OH}$	4.5–7.0
carboxylic acid	RCOOH	9.0–13.0
alkyl amine	$\text{R}-\text{NH}-$	1.0–5.0
aryl amine	$\text{Ar}-\text{NH}_2$	3.0–6.0
amide	RCONHR	5.0–12.0

Note: δ values for O–H and N–H protons can vary depending on solvent and concentration.
Ar is used to represent an aromatic ring.

7 Typical carbon-13 (^{13}C) NMR chemical shift values (δ) relative to TMS = 0

hybridisation of the carbon atom	environment of carbon atom	example	chemical shift range δ/ppm
sp^3	alkyl	CH_3- , CH_2- , $-\text{CH}<$, $>\text{C}<$	0–50
sp^3	next to alkene/arene	$-\text{C}=\text{C}$, $-\text{C}-\text{Ar}$	25–50
sp^3	next to carbonyl/carboxyl	$\text{C}-\text{COR}$, $\text{C}-\text{O}_2\text{R}$	30–65
sp^3	next to halogen	$\text{C}-\text{X}$	30–60
sp^3	next to oxygen	$\text{C}-\text{O}$	50–70
sp^2	alkene or arene	$>\text{C}=\text{C}<$, 	110–160
sp^2	carboxyl	$\text{R}-\text{COOH}$, $\text{R}-\text{COOR}$	160–185
sp^2	carbonyl	$\text{R}-\text{CHO}$, $\text{R}-\text{CO}-\text{R}$	190–220
sp	nitrile	$\text{R}-\text{C}\equiv\text{N}$	100–125

8 Characteristic infrared absorption frequencies for some selected bonds

bond	functional groups containing the bond	characteristic infrared absorption range (in wavenumbers) / cm⁻¹
C–O	hydroxy, ester	1040–1300
C=C	aromatic compound, alkene	1500–1680
C=O	amide carbonyl, carboxyl ester	1640–1690 1670–1740 1710–1750
C≡N	nitrile	2200–2250
C–H	alkane	2850–2950
N–H	amine, amide	3300–3500
O–H	carboxyl hydroxy	2500–3000 3200–3600

9 The Periodic Table of Elements

Group

1	2	13										14	15	16	17	18	
		1															
		H hydrogen 1.0															
Key																	
atomic number atomic symbol name relative atomic mass																	
3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18		
Li lithium 6.9	Be beryllium 9.0									5	6	7	8	9	10		
11	12									13	14	15	16	17	18		
Na sodium 23.0	Mg magnesium 24.3									Al aluminium 27.0	Si silicon 28.1	P phosphorus 31.0	S sulfur 32.1	Cl chlorine 35.5	Ar argon 39.9		
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
K potassium 39.1	Ca calcium 40.1	Sc scandium 45.0	Ti titanium 47.9	V vanadium 50.9	Cr chromium 52.0	Mn manganese 54.9	Fe iron 55.8	Co cobalt 58.9	Ni nickel 58.7	Cu copper 63.5	Zn zinc 65.4	Ga gallium 69.7	Ge germanium 72.6	As arsenic 74.9	Se selenium 79.0	Br bromine 79.9	Kr krypton 83.8
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
Rb rubidium 85.5	Sr strontium 87.6	Y yttrium 88.9	Zr zirconium 91.2	Nb niobium 92.9	Mo molybdenum 95.9	Tc technetium —	Ru ruthenium 101.1	Rh rhodium 102.9	Pd palladium 106.4	Ag silver 107.9	Cd cadmium 112.4	In indium 114.8	Sn tin 118.7	Sb antimony 121.8	Te tellurium 127.6	I iodine 126.9	Xe xenon 131.3
55	56	57–71 lanthanoids	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
Cs caesium 132.9	Ba barium 137.3		Hf hafnium 178.5	Ta tantalum 180.9	W tungsten 183.8	Re rhenium 186.2	Os osmium 190.2	Ir iridium 192.2	Pt platinum 195.1	Au gold 197.0	Hg mercury 200.6	Tl thallium 204.4	Pb lead 207.2	Bi bismuth 209.0	Po polonium —	At astatine —	Rn radon —
87	88	89–103 actinoids	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118
Fr francium —	Ra radium —		Rf rutherfordium —	Db dubnium —	Sg seaborgium —	Bh bohrium —	Hs hassium —	Mt meitnerium —	Ds darmstadtium —	Rg roentgenium —	Cn copernicium —	Nh nihonium —	Fl flerovium —	Mc moscovium —	Lv livermorium —	Ts tennessine —	Og oganeson —
lanthanoids																	
57	58	59	60	61	62	63	64	65	66	67	68	69	70	71			
La lanthanum 138.9	Ce cerium 140.1	Pr praseodymium 140.9	Nd neodymium 144.4	Pm promethium —	Sm samarium 150.4	Eu europium 152.0	Gd gadolinium 157.3	Tb terbium 158.9	Dy dysprosium 162.5	Ho holmium 164.9	Er erbium 167.3	Tm thulium 168.9	Yb ytterbium 173.1	Lu lutetium 175.0			
89	90	91	92	93	94	95	96	97	98	99	100	101	102	103			
Ac actinium —	Th thorium 232.0	Pa protactinium 231.0	U uranium 238.0	Np neptunium —	Pu plutonium —	Am americium —	Cm curium —	Bk berkelium —	Cf californium —	Es einsteinium —	Fm fermium —	Md mendelevium —	No nobelium —	Lr lawrencium —			