Diploma Programme

Chemistry data booklet

First assessment 2016

Edited in 2014 (version 2)

International Baccalaureate®
Baccalauréat International
Bachillerato Internacional

Diploma Programme
Chemistry data booklet

Published June 2014

Published on behalf of the International Baccalaureate Organization, a not-for-profit educational foundation of 15 Route des Morillons, 1218 Le Grand-Saconnex, Geneva, Switzerland by the

International Baccalaureate Organization (UK) Ltd
Peterson House, Malthouse Avenue, Cardiff Gate
Cardiff, Wales CF23 8GL
United Kingdom
Website: www.ibo.org

The International Baccalaureate Organization (known as the IB) offers four high-quality and challenging educational programmes for a worldwide community of schools, aiming to create a better, more peaceful world. This publication is one of a range of materials produced to support these programmes.

The IB may use a variety of sources in its work and checks information to verify accuracy and authenticity, particularly when using community-based knowledge sources such as Wikipedia. The IB respects the principles of intellectual property and makes strenuous efforts to identify and obtain permission before publication from rights holders of all copyright material used. The IB is grateful for permissions received for material used in this publication and will be pleased to correct any errors or omissions at the earliest opportunity.

IB merchandise and publications can be purchased through the IB store at http://store.ibo.org.

Email: sales@ibo.org

Contents

Notes

This booklet cannot be used for paper 1 of the examination (SLP1 and HLP1), but the periodic table given in section 6 will be available as part of these examination papers. Clean copies of this booklet must be made available to candidates for papers 2 and 3 (SLP2, HLP2, SLP3 and HLP3).

1. Some relevant equations

Topic	Equation
1.3	$PV = nRT$
2.2 and C.4	$c = v\lambda$
5.1	$q = mc\Delta T$
8.3	$pH = -\log_{10}[H_3O^+]$ or $pH = -\log_{10}[H^+]$
12.1	$E = hv$
15.2	$\Delta G^\ominus = \Delta H^\ominus - T\Delta S^\ominus$
16.2	$k = Ae^{\frac{-E_a}{RT}}$
16.2	$\ln k = \frac{-E_a}{RT} + \ln A$
16.2	$\ln\frac{k_1}{k_2} = \frac{E_a}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$
17.1	$\Delta G^\ominus = -RT\ln K$
19.1	$\Delta G^\ominus = -nFE^\ominus$
A.5	$\%\text{ atom economy} = \frac{\text{molar mass of desired product}}{\text{molar mass of all reactants}} \times 100$
A.8	$n\lambda = 2d\sin\theta$
B.7	$pH = pK_a + \log\left(\frac{[A^-]}{[HA]}\right)$
B.7	$\log_{10}\frac{I_0}{I} = \varepsilon lc$

Topic	Equation
C.1	$\text{Energy density} = \frac{\text{energy released from fuel}}{\text{volume of fuel consumed}}$
C.1	$\text{Specific energy} = \frac{\text{energy released from fuel}}{\text{mass of fuel consumed}}$
C.3	$N = N_0 e^{-\lambda t}$
C.3 and D.8	$t_{\frac{1}{2}} = \frac{\ln 2}{\lambda}$
C.6	$E = E^0 - \left(\frac{RT}{nF}\right) \ln Q$
C.7	$\frac{\text{Rate}_1}{\text{Rate}_2} = \sqrt{\frac{M_2}{M_1}}$
D.8	$N_t = N_0(0.5)^{t/k}$

2. Physical constants and unit conversions

Avogadro's constant (L or N_A) $= 6.02 \times 10^{23}$ mol^{-1}

Gas constant (R) $= 8.31$ J K^{-1} mol^{-1}

Molar volume of an ideal gas at STP $= 2.27 \times 10^{-2}$ m^3 mol^{-1} $= 22.7$ dm^3 mol^{-1}

1 dm^3 $= 1$ litre $= 1 \times 10^{-3}$ m^3 $= 1 \times 10^3$ cm^3

STP conditions $= 273$ K and 100 kPa

SATP conditions $= 298$ K and 100 kPa

Speed of light $= 3.00 \times 10^8$ ms^{-1}

Specific heat capacity of water $= 4.18$ kJ kg^{-1}K^{-1} $= 4.18$ J g^{-1} K^{-1}

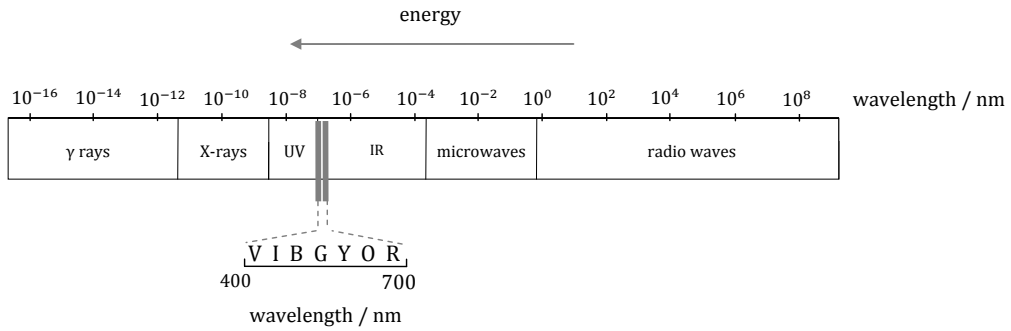
Planck's constant (h) $= 6.63 \times 10^{-34}$ J s

Faraday's constant (F) $= 9.65 \times 10^4$ C mol^{-1}

Ionic product constant for water (K_w) $= 1.00 \times 10^{-14}$ mol^2 dm^{-6} at 298 K

1 amu $= 1.66 \times 10^{-27}$ kg

3. The electromagnetic spectrum



4. Fundamental particles

	Proton	Neutron	Electron
Mass (kg)	1.672622×10^{-27}	1.674927×10^{-27}	9.109383×10^{-31}
Charge (C)	1.602189×10^{-19}	0	$-1.602189 \times 10^{-19}$

5. Names of the elements

Element	Symbol	Atomic number
actinium	Ac	89
aluminium	Al	13
americium	Am	95
antimony	Sb	51
argon	Ar	18
arsenic	As	33
astatine	At	85
barium	Ba	56
berkelium	Bk	97
beryllium	Be	4
bismuth	Bi	83
bohrium	Bh	107
boron	B	5
bromine	Br	35
cadmium	Cd	48
caesium	Cs	55
calcium	Ca	20
californium	Cf	98
carbon	C	6
cerium	Ce	58
chlorine	Cl	17
chromium	Cr	24
cobalt	Co	27
copernicium	Cn	112
copper	Cu	29
curium	Cm	96
darmstadtium	Ds	110
dubnium	Db	105

Element	Symbol	Atomic number
dysprosium	Dy	66
einsteinium	Es	99
erbium	Er	68
europium	Eu	63
fermium	Fm	100
fluorine	F	9
francium	Fr	87
gadolinium	Gd	64
gallium	Ga	31
germanium	Ge	32
gold	Au	79
hafnium	Hf	72
hassium	Hs	108
helium	He	2
holmium	Ho	67
hydrogen	H	1
indium	In	49
iodine	I	53
iridium	Ir	77
iron	Fe	26
krypton	Kr	36
lanthanum	La	57
lawrencium	Lr	103
lead	Pb	82
lithium	Li	3
lutetium	Lu	71
magnesium	Mg	12
manganese	Mn	25

Element	Symbol	Atomic number
meitnerium	Mt	109
mendelevium	Md	101
mercury	Hg	80
molybdenum	Mo	42
neodymium	Nd	60
neon	Ne	10
neptunium	Np	93
nickel	Ni	28
niobium	Nb	41
nitrogen	N	7
nobelium	No	102
osmium	Os	76
oxygen	O	8
palladium	Pd	46
phosphorus	P	15
platinum	Pt	78
plutonium	Pu	94
polonium	Po	84
potassium	K	19
praseodymium	Pr	59
promethium	Pm	61
protactinium	Pa	91
radium	Ra	88
radon	Rn	86
rhenium	Re	75
rhodium	Rh	45
roentgenium	Rg	111
rubidium	Rb	37

Element	Symbol	Atomic number
ruthenium	Ru	44
rutherfordium	Rf	104
samarium	Sm	62
scandium	Sc	21
seaborgium	Sg	106
selenium	Se	34
silicon	Si	14
silver	Ag	47
sodium	Na	11
strontium	Sr	38
sulfur	S	16
tantalum	Ta	73
technetium	Tc	43
tellurium	Te	52
terbium	Tb	65
thallium	Tl	81
thorium	Th	90
thulium	Tm	69
tin	Sn	50
titanium	Ti	22
tungsten	W	74
uranium	U	92
vanadium	V	23
xenon	Xe	54
ytterbium	Yb	70
yttrium	Y	39
zinc	Zn	30
zirconium	Zr	40

6. The periodic table

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 **H** 1.01						Atomic number **Element** Relative atomic mass											2 **He** 4.00
2	3 **Li** 6.94	4 **Be** 9.01											5 **B** 10.81	6 **C** 12.01	7 **N** 14.01	8 **O** 16.00	9 **F** 19.00	10 **Ne** 20.18
3	11 **Na** 22.99	12 **Mg** 24.31											13 **Al** 26.98	14 **Si** 28.09	15 **P** 30.97	16 **S** 32.07	17 **Cl** 35.45	18 **Ar** 39.95
4	19 **K** 39.10	20 **Ca** 40.08	21 **Sc** 44.96	22 **Ti** 47.87	23 **V** 50.94	24 **Cr** 52.00	25 **Mn** 54.94	26 **Fe** 55.85	27 **Co** 58.93	28 **Ni** 58.69	29 **Cu** 63.55	30 **Zn** 65.38	31 **Ga** 69.72	32 **Ge** 72.63	33 **As** 74.92	34 **Se** 78.96	35 **Br** 79.90	36 **Kr** 83.90
5	37 **Rb** 85.47	38 **Sr** 87.62	39 **Y** 88.91	40 **Zr** 91.22	41 **Nb** 92.91	42 **Mo** 95.96	43 **Tc** (98)	44 **Ru** 101.07	45 **Rh** 102.91	46 **Pd** 106.42	47 **Ag** 107.87	48 **Cd** 112.41	49 **In** 114.82	50 **Sn** 118.71	51 **Sb** 121.76	52 **Te** 127.60	53 **I** 126.90	54 **Xe** 131.29
6	55 **Cs** 132.91	56 **Ba** 137.33	57 † **La** 138.91	72 **Hf** 178.49	73 **Ta** 180.95	74 **W** 183.84	75 **Re** 186.21	76 **Os** 190.23	77 **Ir** 192.22	78 **Pt** 195.08	79 **Au** 196.97	80 **Hg** 200.59	81 **Tl** 204.38	82 **Pb** 207.20	83 **Bi** 208.98	84 **Po** (209)	85 **At** (210)	86 **Rn** (222)
7	87 **Fr** (223)	88 **Ra** (226)	89 ‡ **Ac** (227)	104 **Rf** (267)	105 **Db** (268)	106 **Sg** (269)	107 **Bh** (270)	108 **Hs** (269)	109 **Mt** (278)	110 **Ds** (281)	111 **Rg** (281)	112 **Cn** (285)	113 **Uut** (286)	114 **Uuq** (289)	115 **Uup** (288)	116 **Uuh** (293)	117 **Uus** (294)	118 **Uuo** (294)

†	58 **Ce** 140.12	59 **Pr** 140.91	60 **Nd** 144.24	61 **Pm** (145)	62 **Sm** 150.36	63 **Eu** 151.96	64 **Gd** 157.25	65 **Tb** 158.93	66 **Dy** 162.50	67 **Ho** 164.93	68 **Er** 167.26	69 **Tm** 168.93	70 **Yb** 173.05	71 **Lu** 174.97
‡	90 **Th** 232.04	91 **Pa** 231.04	92 **U** 238.03	93 **Np** (237)	94 **Pu** (244)	95 **Am** (243)	96 **Cm** (247)	97 **Bk** (247)	98 **Cf** (251)	99 **Es** (252)	100 **Fm** (257)	101 **Md** (258)	102 **No** (259)	103 **Lr** (262)

7. Melting points and boiling points of the elements (at 101.325 kPa)

−259.2 **H** −252.9						Melting point (°C) **Element** Boiling point (°C)											**He** −268.9
180.5 **Li** 1342	1287 **Be** 2468											2077 **B** 4000	3500 **C** 4827	−210.0 **N** −195.8	−218.8 **O** −183.0	−219.7 **F** −188.1	−248.6 **Ne** −246.0
97.79 **Na** 882.9	650.0 **Mg** 1090											660.3 **Al** 2519	1414 **Si** 3265	44.15 **P** 280.5	115.2 **S** 444.6	−101.5 **Cl** −34.04	−189.3 **Ar** −185.8
63.38 **K** 758.8	842.0 **Ca** 1484	1541 **Sc** 2836	1670 **Ti** 3287	1910 **V** 3407	1907 **Cr** 2671	1246 **Mn** 2061	1538 **Fe** 2861	1495 **Co** 2927	1455 **Ni** 2913	1085 **Cu** 2560	419.5 **Zn** 907.0	29.77 **Ga** 2229	938.2 **Ge** 2833	816.8 **As** 613.0	220.8 **Se** 684.8	−7.050 **Br** 58.78	−157.4 **Kr** −153.4
39.30 **Rb** 687.8	768.8 **Sr** 1377	1522 **Y** 3345	1854 **Zr** 4406	2477 **Nb** 4741	2622 **Mo** 4639	2157 **Tc** 4262	2333 **Ru** 4147	1963 **Rh** 3695	1555 **Pd** 2963	961.8 **Ag** 2162	321.1 **Cd** 766.8	156.6 **In** 2027	231.9 **Sn** 2586	630.6 **Sb** 1587	449.5 **Te** 987.8	113.7 **I** 184.4	−111.8 **Xe** −108.1
28.44 **Cs** 670.8	725.0 **Ba** 1845	920.0 **La** 3464	2233 **Hf** 4600	3017 **Ta** 5455	3414 **W** 5555	3453 **Re** 5900	3033 **Os** 5008	2446 **Ir** 4428	1768 **Pt** 3825	1064 **Au** 2836	−38.83 **Hg** 356.6	303.8 **Tl** 1473	327.5 **Pb** 1749	271.4 **Bi** 1564	253.8 **Po** 962.0	301.8 **At** 336.8	−71.15 **Rn** −61.85
27.00 **Fr** 676.8	699.8 **Ra** 1140	1050 **Ac** 3200															

8. First ionization energy, electron affinity and electronegativity of the elements

1312 −73 **H** 2.2																	2372 **He**
520 −60 **Li** 1.0	900 **Be** 1.6											801 −27 **B** 2.0	1086 −122 **C** 2.6	1402 **N** 3.0	1314 −141 (+753) **O** 3.4	1681 −328 **F** 4.0	2081 **Ne**
496 −53 **Na** 0.9	738 **Mg** 1.3											578 −42 **Al** 1.6	787 −134 **Si** 1.9	1012 −72 **P** 2.2	1000 −200 (+545) **S** 2.6	1251 −349 **Cl** 3.2	1520 **Ar**
419 −48 **K** 0.8	590 −2 **Ca** 1.0	633 −18 **Sc** 1.4	659 −8 **Ti** 1.5	651 −51 **V** 1.6	653 −64 **Cr** 1.7	717 **Mn** 1.6	762 −15 **Fe** 1.8	760 −64 **Co** 1.9	737 −112 **Ni** 1.9	745 −119 **Cu** 1.9	906 **Zn** 1.6	579 −41 **Ga** 1.8	762 −119 **Ge** 2.0	944 −78 **As** 2.2	941 −195 **Se** 2.6	1140 −325 **Br** 3.0	1351 **Kr**
403 −47 **Rb** 0.8	549 −5 **Sr** 1.0	600 −30 **Y** 1.2	640 −41 **Zr** 1.3	652 −88 **Nb** 1.6	684 −72 **Mo** 2.2	702 −53 **Tc** 2.1	710 −101 **Ru** 2.2	720 −110 **Rh** 2.3	804 −54 **Pd** 2.2	731 −126 **Ag** 1.9	868 **Cd** 1.7	558 −29 **In** 1.8	709 −107 **Sn** 2.0	831 −101 **Sb** 2.0	869 −190 **Te** 2.1	1008 −295 **I** 2.7	1170 **Xe** 2.6
376 −46 **Cs** 0.8	503 −14 **Ba** 0.9	538 −45 **La** 1.1	659 −1 **Hf** 1.3	728 −31 **Ta** 1.5	759 −79 **W** 1.7	756 −14 **Re** 1.9	814 −106 **Os** 2.2	865 −151 **Ir** 2.2	864 −205 **Pt** 2.2	890 −223 **Au** 2.4	1007 **Hg** 1.9	589 −36 **Tl** 1.8	716 −35 **Pb** 1.8	703 −91 **Bi** 1.9	812 −183 **Po** 2.0	−270 **At** 2.2	1037 **Rn**
393 −47 **Fr** 0.7	509 −10 **Ra** 0.9	499 −34 **Ac** 1.1															

First ionization energy (kJ mol⁻¹) — Electron affinity (kJ mol⁻¹) (2nd EA / kJ mol⁻¹)

Element

Electronegativity

9. Atomic and ionic radii of the elements

32 **H**																	37 **He**
130 **Li** 76 (1+)	99 **Be** 45 (2+)											84 **B** 27 (3+)	75 **C** 16 (4+)	71 **N** 146 (3−)	64 **O** 140 (2−)	60 **F** 133 (1−)	62 **Ne**
160 **Na** 102 (1+)	140 **Mg** 72 (2+)											124 **Al** 54 (3+)	114 **Si** 40 (4+)	109 **P** 38 (5+)	104 **S** 184 (2−)	100 **Cl** 181 (1−)	101 **Ar**
200 **K** 138 (1+)	174 **Ca** 100 (2+)	159 **Sc** 75 (3+)	148 **Ti** 86 (2+) 61 (4+)	144 **V** 79 (2+) 54 (5+)	130 **Cr** 62 (3+) 44 (6+)	129 **Mn** 83 (2+) 53 (4+)	124 **Fe** 61 (2+) 55 (3+)	118 **Co** 65(+2) 55 (+3)	117 **Ni** 69 (2+)	122 **Cu** 77 (1+) 73 (2+)	120 **Zn** 74 (2+)	123 **Ga** 62(3+)	120 **Ge** 53 (4+) 272(4−)	120 **As** 58 (3+) 46 (5+)	118 **Se** 198 (2−)	117 **Br** 196 (1−)	116 **Kr**
215 **Rb** 152 (1+)	190 **Sr** 118 (2+)	176 **Y** 90 (3+)	164 **Zr** 72 (4+)	156 **Nb** 72 (3+) 64 (5+)	146 **Mo** 65 (4+)	138 **Tc** 65(4+)	136 **Ru** 68(3+) 62 (4+)	134 **Rh** 67 (+3) 60 (+4)	130 **Pd** 86(2+) 62(4+)	136 **Ag** 115 (1+)	140 **Cd** 95 (2+)	142 **In** 80(3+)	140 **Sn** 118(2+) 69 (4+)	140 **Sb** 76 (3+)	137 **Te** 221 (2−)	136 **I** 220(1−)	136 **Xe**
238 **Cs** 167 (1+)	206 **Ba** 135 (2+)	194 **La** 103 (3+)	164 **Hf** 71 (4+)	158 **Ta** 64 (5+)	150 **W** 66 (4+) 60(6+)	141 **Re** 63(4+) 53(7+)	136 **Os** 63 (4+) 55(6+)	132 **Ir** 68(+3) 63 (+4)	130 **Pt** 80(2+) 63(4+)	130 **Au** 137 (1+) 85 (3+)	132 **Hg** 119 (1+) 102 (2+)	144 **Tl** 150 (1+) 89 (3)	145 **Pb** 119 (2+) 78 (4+)	150 **Bi** 103 (3+) 76(5+)	142 **Po** 97(4+)	148 **At**	146 **Rn**
242 **Fr**	211 **Ra**	201 **Ac**															

Atomic radius
(10^{-12} m)

Element

Ionic radius
(10^{-12} m)

10. Covalent bond lengths

Single bonds (10^{-12}m = pm)

	Br	C	Cl	F	H	I	N	O	P	S	Si
Br	228	194	214	176	141	247	214		220	227	216
C	194	154	177	138	108	214	147	143	184	182	185
Cl	214	177	199	163	128	232	197	170	203	199	202
F	176	138	163	142	92	257	136	142	154	158	156
H	141	108	128	92	74	160	101	97	142	134	148
I	247	214	232	257	160	267			247		243
N	214	147	197	136	101		146	136		175	174
O		143	170	142	97		136	148	154	161	163
P	220	184	203	154	142	247		154	221	210	
S	227	182	199	158	134		175	161	210	205	215
Si	216	185	202	156	148	243	174	163		215	232

Multiple bonds (10^{-12}m = pm)

C=C	134	C≡N	116	N≡N	110
C≡C	120	C=O	122	N=O	114
C⎓C (in benzene)	140	C=S	156	O=O	121
C=N	130	N=N	125	S=S	189

11. Bond enthalpies and average bond enthalpies at 298 K

Single bonds (kJ mol^{-1})

	Br	C	Cl	F	H	I	N	O	P	S	Si
Br	193	285	219	249	366	178		201	264	218	330
C	285	346	324	492	414	228	286	358	264	289	307
Cl	219	324	242	255	431	211	192	206	322	271	400
F	249	492	255	159	567	280	278	191	490	327	597
H	366	414	431	567	436	298	391	463	322	364	323
I	178	228	211	280	298	151		201	184		234
N		286	192	278	391		158	214			
O	201	358	206	191	463	201	214	144	363		466
P	264	264	322	490	322	184		363	198		
S	218	289	271	327	364					266	293
Si	330	307	400	597	323	234		466		293	226

Multiple bonds (kJ mol^{-1})

C=C	614	C≡N	890	N≡N	945
C≡C	839	C=O	804	N=O	587
C⩵C (in benzene)	507	C=S	536	O=O	498
C=N	615	N=N	470	S=S	429

12. Selected compounds—thermodynamic data

Substance	Formula	State	$\Delta H_f^\ominus$ (kJ mol^{-1})	$\Delta G_f^\ominus$ (kJ mol^{-1})	$S^\ominus$ (J K^{-1} mol^{-1})
methane	CH_4	g	−74.0	−50.0	+186
ethane	C_2H_6	g	−84.0	−32.0	+230
propane	C_3H_8	g	−105	−24.0	+270
butane	C_4H_{10}	g	−126	−17.0	+310
pentane	C_5H_{12}	l	−173		
hexane	C_6H_{14}	l	−199		
ethene	C_2H_4	g	+52.0	+68.0	+220
propene	C_3H_6	g	+20.0	+62.0	+267
but-1-ene	C_4H_8	g	+0.10	+71.0	+306
cis-but-2-ene	C_4H_8	g	−7.0	+66.0	+301
trans-but-2-ene	C_4H_8	g	−11.0	+63.0	+297
ethyne	C_2H_2	g	+228	+211	+201
propyne	C_3H_4	g	+185	+194	+248
buta-1,3-diene	C_4H_6	g	+110	+151	+279
cyclohexane	C_6H_{12}	l	−156		
benzene	C_6H_6	l	+49.0	+125	+173
methylbenzene	$C_6H_5CH_3$	l	+12.0		
ethylbenzene	$C_6H_5CH_2CH_3$	l	−12.0		
phenylethene	$C_6H_5CHCH_2$	l	+104		
chloromethane	CH_3Cl	g	−82.0	−58.0	+235
dichloromethane	CH_2Cl_2	l	−124		+178
trichloromethane	$CHCl_3$	l	−134	−74.0	+202
bromomethane	CH_3Br	g	−36.0	−26.0	+246
iodomethane	CH_3I	l	−14.0		+163
chloroethane	C_2H_5Cl	g	−137	−53.0	
bromoethane	C_2H_5Br	l	−90.0	−26.0	+199
chlorobenzene	C_6H_5Cl	l	+11.0		
methanol	CH_3OH	l	−239	−167	+127
ethanol	C_2H_5OH	l	−278	−175	+161
phenol	C_6H_5OH	s	−165		+144
methanal	$HCHO$	g	−109	−102	+219
ethanal	CH_3CHO	g	−166	−133	+264
propanone	$(CH_3)_2CO$	l	−248		+200
methanoic acid	$HCOOH$	l	−425	−361	+129
ethanoic acid	CH_3COOH	l	−484	−390	+160
benzoic acid	C_6H_5COOH	s	−385		+168
methylamine	CH_3NH_2	g	−23	+32.0	+243
water	H_2O	l	−285.8	−237.1	+70.0
steam	H_2O	g	−241.8	−228.6	+188.8
carbon monoxide	CO	g	−110.5	−137.2	+197.7
carbon dioxide	CO_2	g	−393.5	−394.4	+213.8
hydrogen bromide	HBr	g	−36.3	−53.4	+198.7
hydrogen chloride	HCl	g	−92.3	−95.3	+186.9
hydrogen fluoride	HF	g	−273.3	−275.4	+173.8
hydrogen iodide	HI	g	+26.5	+1.7	+206.6

13. Enthalpies of combustion

The values of the molar enthalpy of combustion($\Delta H_c^{\ominus}$) in the following table refer to a temperature of 298 K and a pressure of 1.00×10^5 Pa .

Substance	Formula	State	$\Delta H_c^{\ominus}$ (kJ mol^{-1})
hydrogen	H_2	g	−286
sulfur	S	s	−297
carbon (graphite)	C	s	−394
carbon monoxide	CO	g	−283
methane	CH_4	g	−891
ethane	C_2H_6	g	−1561
propane	C_3H_8	g	−2219
butane	C_4H_{10}	g	−2878
pentane	C_5H_{12}	l	−3509
hexane	C_6H_{14}	l	−4163
octane	C_8H_{18}	l	−5470
cyclohexane	C_6H_{12}	l	−3920
ethene	C_2H_4	g	−1411
buta-1,3-diene	C_4H_6	g	−2541
ethyne	C_2H_2	g	−1301
benzene	C_6H_6	l	−3268
methylbenzene	$C_6H_5CH_3$	l	−3910
naphthalene	$C_{10}H_8$	s	−5156
chloroethane	C_2H_5Cl	g	−1413
iodoethane	C_2H_5I	l	−1463
trichloromethane	$CHCl_3$	l	−473
methanol	CH_3OH	l	−726
ethanol	C_2H_5OH	l	−1367

Substance	Formula	State	$\Delta H_c^{\ominus}$ (kJ mol^{-1})
propan-1-ol	C_3H_7OH	l	−2021
butan-1-ol	C_4H_9OH	l	−2676
cyclohexanol	$C_6H_{11}OH$	s	−3728
phenol	C_6H_5OH	s	−3053
ethoxyethane	$(C_2H_5)_2O$	l	−2724
methanal	HCHO	g	−571
ethanal	CH_3CHO	g	−1167
benzaldehyde	C_6H_5CHO	l	−3525
propanone	$(CH_3)_2CO$	l	−1790
pentan-3-one	$(C_2H_5)_2CO$	l	−3100
phenylethanone	$CH_3COC_6H_5$	l	−4149
methanoic acid	HCOOH	l	−255
ethanoic acid	CH_3COOH	l	−874
benzoic acid	C_6H_5COOH	s	−3228
ethanedioic acid	$(COOH)_2$	s	−243
ethyl ethanoate	$CH_3COOC_2H_5$	l	−2238
ethanamide	CH_3CONH_2	s	−1186
methylamine	CH_3NH_2	g	−1086
phenylamine	$C_6H_5NH_2$	l	−3393
nitrobenzene	$C_6H_5NO_2$	l	−3088
urea	$CO(NH_2)_2$	s	−633
glucose	$C_6H_{12}O_6$	s	−2803
sucrose	$C_{12}H_{22}O_{11}$	s	−5640

14. Common oxidation numbers of the 3d ions

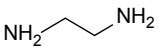
Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
								+1	
	+2	+2	+2	+2	+2	+2	+2	+2	+2
+3	+3	+3	+3	+3	+3	+3			
	+4	+4		+4					
		+5							
			+6	+6					
				+7					

15. Spectrochemical series

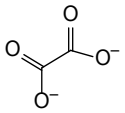
Ligands can be arranged in a spectrochemical series according to the energy difference they produce between the two sets of d-orbitals in an octahedral complex.

$$I^- < Br^- < S^{2-} < Cl^- < F^- < OH^- < H_2O < SCN^- < NH_3 < CN^- \approx CO$$

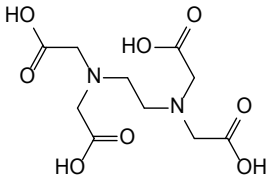
16. Ligands



1,2-ethanediamine

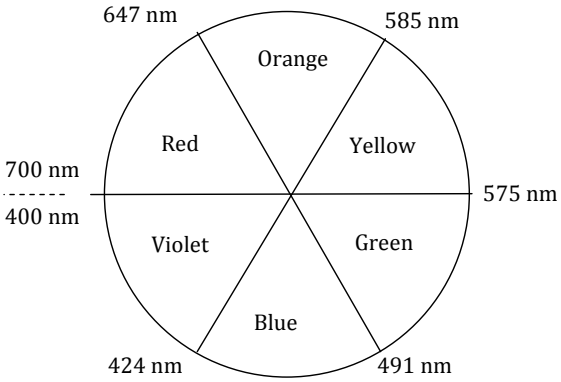


ethanedioate



EDTA

17. Colour wheel



18. Lattice enthalpies at 298 K (experimental values)

The lattice enthalpy values ($\Delta H^{\ominus}_{\text{lattice}}$) given relate to the endothermic process $M_aX_b(s) \rightarrow aM^{b+}(g) + bX^{a-}(g)$ in which the gaseous ions of a crystal are separated to an infinite distance from each other.

Experimental values

The data in these tables are experimental values obtained by means of a suitable Born–Haber cycle.

Alkali metal halides	$\Delta H^{\ominus}_{\text{lattice}}$ (kJ mol^{-1})			
	F	Cl	Br	I
Li	1049	864	820	764
Na	930	790	754	705
K	829	720	691	650
Rb	795	695	668	632
Cs	759	670	647	613

Other substances	$\Delta H^{\ominus}_{\text{lattice}}$ (kJ mol^{-1})
CaF_2	2651
$BeCl_2$	3033
$MgCl_2$	2540
$CaCl_2$	2271
$SrCl_2$	2170
$BaCl_2$	2069
MgO	3791
CaO	3401

Other substances	$\Delta H^{\ominus}_{\text{lattice}}$ (kJ mol^{-1})
SrO	3223
BaO	3054
$CuCl_2$	2824
AgF	974
AgCl	918
AgBr	905
AgI	892

19. Enthalpies of aqueous solutions

Solute	$\Delta H^{\ominus}_{sol}$ (kJ mol^{-1})
NH_4Cl	+14.78
NH_4NO_3	+25.69
LiF	+4.73
LiCl	−37.03
LiBr	−48.83
LiI	−63.30
NaF	+0.91
NaCl	+3.88
NaBr	−0.60
NaI	−7.53
KF	−17.73

Solute	$\Delta H^{\ominus}_{sol}$ (kJ mol^{-1})
KCl	+17.22
KBr	+19.87
KI	+20.33
RbF	−26.11
RbCl	+17.28
RbBr	+21.88
RbI	+25.10
CsF	−36.86
CsCl	+17.78
CsBr	+25.98
CsI	+33.35

20. Enthalpies of hydration

Cations	$\Delta H^{\ominus}_{hyd}$ (kJ mol^{-1})
Li^+	−538
Na^+	−424
K^+	−340
Rb^+	−315
Cs^+	−291
Be^{2+}	−2524
Mg^{2+}	−1963
Ca^{2+}	−1616
Sr^{2+}	−1483
Ba^{2+}	−1346
Ra^{2+}	−1335
Al^{3+}	−4741
Ga^{3+}	−4745
In^{3+}	−4171
Tl^{3+}	−4163
Tl^+	−346
Sn^{2+}	−1587
Pb^{2+}	−1523

Anions	$\Delta H^{\ominus}_{hyd}$ (kJ mol^{-1})
F^-	−504
Cl^-	−359
Br^-	−328
I^-	−287
ClO_3^-	−331
BrO_3^-	−358
IO_3^-	−446
ClO_4^-	−205
OH^-	−519
CN^-	−341
NO_3^-	−316
HCO_3^-	−383
CO_3^{2-}	−1486
HSO_4^-	−362
SO_4^{2-}	−1099
PO_4^{3-}	−2921

21. Strengths of organic acids and bases

The acid strengths in the following tables are given in terms of pK_a values, where $pK_a = -\log_{10}K_a$.

The dissociation constant K_a values are for aqueous solutions at 298 K. Base strengths are given in terms of pK_b values.

Carboxylic acids

Name	Formula	pK_a
methanoic	$HCOOH$	3.75
ethanoic	CH_3COOH	4.76
propanoic	CH_3CH_2COOH	4.87
butanoic	$CH_3(CH_2)_2COOH$	4.83
2-methylpropanoic	$(CH_3)_2CHCOOH$	4.84
pentanoic	$CH_3(CH_2)_3COOH$	4.83
2,2-dimethylpropanoic	$(CH_3)_3CCOOH$	5.03
benzoic	C_6H_5COOH	4.20
phenylethanoic	$C_6H_5CH_2COOH$	4.31

Halogenated carboxylic acids

Name	Formula	pK_a
chloroethanoic	$CH_2ClCOOH$	2.87
dichloroethanoic	$CHCl_2COOH$	1.35
trichloroethanoic	CCl_3COOH	0.66
fluoroethanoic	CH_2FCOOH	2.59
bromoethanoic	$CH_2BrCOOH$	2.90
iodoethanoic	CH_2ICOOH	3.18

Phenols

Name	Formula	pK_a
phenol	C_6H_5OH	9.99
2-nitrophenol	$O_2NC_6H_4OH$	7.23
3-nitrophenol	$O_2NC_6H_4OH$	8.36
4-nitrophenol	$O_2NC_6H_4OH$	7.15
2,4-dinitrophenol	$(O_2N)_2C_6H_3OH$	4.07
2,4,6-trinitrophenol	$(O_2N)_3C_6H_2OH$	0.42

Alcohols

Name	Formula	pK_a
methanol	CH_3OH	15.5
ethanol	C_2H_5OH	15.5

Amines

Name	Formula	pK_b
ammonia	NH_3	4.75
methylamine	CH_3NH_2	3.34
ethylamine	$CH_3CH_2NH_2$	3.35
dimethylamine	$(CH_3)_2NH$	3.27
trimethylamine	$(CH_3)_3N$	4.20
diethylamine	$(C_2H_5)_2NH$	3.16
triethylamine	$(C_2H_5)_3N$	3.25
phenylamine	$C_6H_5NH_2$	9.13

22. Acid-base indicators

			Colour change	
Indicator	**pK_a**	**pH range**	**Acid**	**Alkali**
methyl orange	3.7	3.1–4.4	red	yellow
bromophenol blue	4.2	3.0–4.6	yellow	blue
bromocresol green	4.7	3.8–5.4	yellow	blue
methyl red	5.1	4.4–6.2	red	yellow
bromothymol blue	7.0	6.0–7.6	yellow	blue
phenol red	7.9	6.8–8.4	yellow	red
phenolphthalein	9.6	8.3–10.0	colourless	pink

23. Values of the ionization constant of water

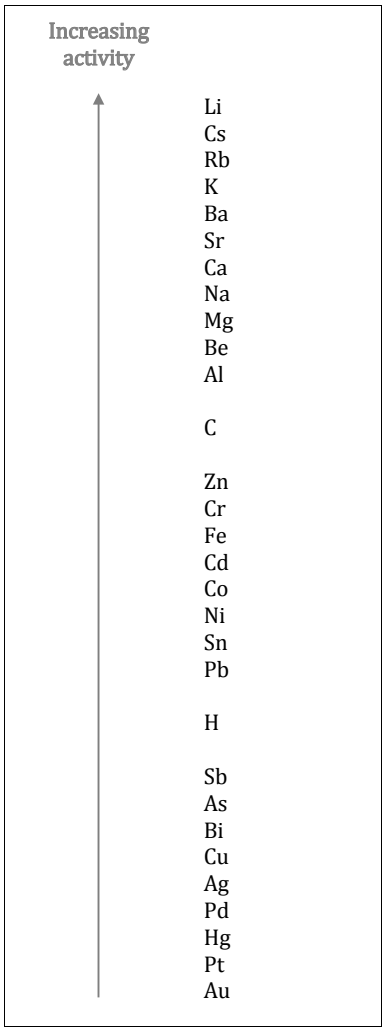
Temperature (°C)	K_w value
0	0.113×10^{-14}
5	0.185×10^{-14}
10	0.292×10^{-14}
15	0.453×10^{-14}
20	0.684×10^{-14}
25	1.00×10^{-14}
30	1.47×10^{-14}
35	2.09×10^{-14}
40	2.92×10^{-14}
45	4.02×10^{-14}
50	5.43×10^{-14}
55	7.24×10^{-14}
60	9.55×10^{-14}
65	12.4×10^{-14}
70	15.9×10^{-14}
75	20.1×10^{-14}
80	25.2×10^{-14}
85	31.3×10^{-14}
90	38.3×10^{-14}
95	46.6×10^{-14}
100	56.0×10^{-14}

24. Standard electrode potentials at 298 K

Oxidized species	⇌	Reduced species	$E^{\ominus}$(V)
$Li^+(aq) + e^-$	⇌	$Li(s)$	−3.04
$K^+(aq) + e^-$	⇌	$K(s)$	−2.93
$Ca^{2+}(aq) + 2e^-$	⇌	$Ca(s)$	−2.87
$Na^+(aq) + e^-$	⇌	$Na(s)$	−2.71
$Mg^{2+}(aq) + 2e^-$	⇌	$Mg(s)$	−2.37
$Al^{3+}(aq) + 3e^-$	⇌	$Al(s)$	−1.66
$Mn^{2+}(aq) + 2e^-$	⇌	$Mn(s)$	−1.18
$H_2O(l) + e^-$	⇌	$\frac{1}{2}H_2(g) + OH^-(aq)$	−0.83
$Zn^{2+}(aq) + 2e^-$	⇌	$Zn(s)$	−0.76
$Fe^{2+}(aq) + 2e^-$	⇌	$Fe(s)$	−0.45
$Ni^{2+}(aq) + 2e^-$	⇌	$Ni(s)$	−0.26
$Sn^{2+}(aq) + 2e^-$	⇌	$Sn(s)$	−0.14
$Pb^{2+}(aq) + 2e^-$	⇌	$Pb(s)$	−0.13
$H^+(aq) + e^-$	⇌	$\frac{1}{2}H_2(g)$	0.00

Oxidized species	⇌	Reduced species	$E^{\ominus}$(V)
$Cu^{2+}(aq) + e^-$	⇌	$Cu^+(aq)$	+0.15
$SO_4^{2-}(aq) + 4H^+(aq) + 2e^-$	⇌	$H_2SO_3(aq) + H_2O(l)$	+0.17
$Cu^{2+}(aq) + 2e^-$	⇌	$Cu(s)$	+0.34
$\frac{1}{2}O_2(g) + H_2O(l) + 2e^-$	⇌	$2OH^-(aq)$	+0.40
$Cu^+(aq) + e^-$	⇌	$Cu(s)$	+0.52
$\frac{1}{2}I_2(s) + e^-$	⇌	$I^-(aq)$	+0.54
$Fe^{3+}(aq) + e^-$	⇌	$Fe^{2+}(aq)$	+0.77
$Ag^+(aq) + e^-$	⇌	$Ag(s)$	+0.80
$\frac{1}{2}Br_2(l) + e^-$	⇌	$Br^-(aq)$	+1.09
$\frac{1}{2}O_2(g) + 2H_2(aq) + 2e^-$	⇌	$H_2O(l)$	+1.23
$Cr_2O_7^{2-}(aq) + 14H^+(aq) + 6e^-$	⇌	$2Cr^{3+}(aq) + 7H_2O(l)$	+1.36
$\frac{1}{2}Cl_2(g) + e^-$	⇌	$Cl^-(aq)$	+1.36
$MnO_4^-(aq) + 8H^+(aq) + 5e^-$	⇌	$Mn^{2+} + 4H_2O(l)$	+1.51
$\frac{1}{2}F_2(g) + e^-$	⇌	$F^-(aq)$	+2.87

25. Activity series



26. Infrared data

Characteristic ranges for infrared absorption due to stretching vibrations in organic molecules.

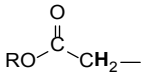
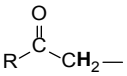
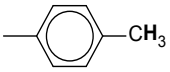
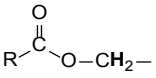
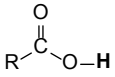
Bond	Organic molecules	Wavenumber (cm^{-1})	Intensity
C–I	iodoalkanes	490–620	strong
C–Br	bromoalkanes	500–600	strong
C–Cl	chloroalkanes	600–800	strong
C–F	fluoroalkanes	1000–1400	strong
C–O	alcohols, esters, ethers	1050–1410	strong
C=C	alkenes	1620–1680	medium-weak; multiple bands
C=O	aldehydes, ketones, carboxylic acids and esters	1700–1750	strong
C≡C	alkynes	2100–2260	variable
O–H	hydrogen bonding in carboxylic acids	2500–3000	strong, very broad
C–H	alkanes, alkenes, arenes	2850–3090	strong
O–H	hydrogen bonding in alcohols and phenols	3200–3600	strong, broad
N–H	primary amines	3300–3500	medium, two bands

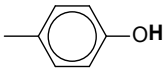
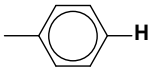
27. ^{1}H NMR data

Typical proton chemical shift values (δ) relative to tetramethylsilane (TMS) = 0 .

R represents an alkyl group, and Hal represents F, Cl, Br, or I.

These values may vary in different solvents and conditions.

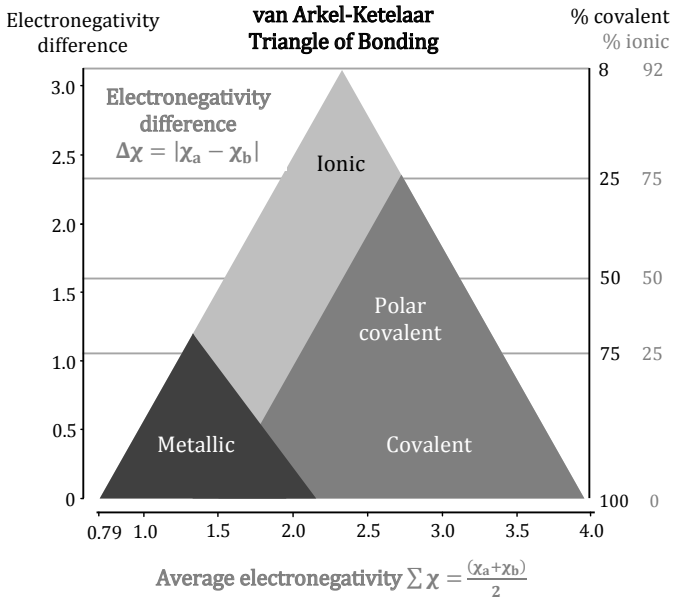
Type of proton	Chemical shift (ppm)
—C**H**$_3$	0.9–1.0
—C**H**$_2$-R	1.3–1.4
—R$_2$C**H**	1.5
	2.0–2.5
	2.2–2.7
	2.5–3.5
—C≡C—**H**	1.8–3.1
—C**H**$_2$-Hal	3.5–4.4
R—O—C**H**$_2$—	3.3–3.7
	3.7–4.8
	9.0–13.0
R—O—**H**	1.0–6.0
—HC=C**H**$_2$	4.5–6.0

Type of proton	Chemical shift (ppm)
	4.0–12.0
	6.9–9.0
	9.4–10.0

28. Mass spectral fragments lost

Mass lost	Fragment lost
15	CH_3
17	OH
18	H_2O
28	$CH_2{=}CH_2$, C=O
29	CH_3CH_2 , CHO
31	CH_3O
45	COOH

29. Triangular bonding diagram

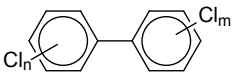


30. Resin identification codes

Resin Identification Code (RIC)	Plastic types
1 PETE	polyethylene terephthalate
2 HDPE	high-density polyethylene
3 PVC	polyvinyl chloride
4 LDPE	low-density polyethylene

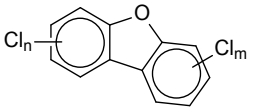
Resin Identification Code (RIC)	Plastic types
5 PP	polypropylene
6 PS	polystyrene
7 OTHER	other

31. Representations of some materials molecules

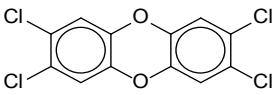


polychlorinated biphenyls

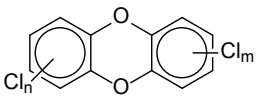
1,4-dioxin



polychlorinated dibenzofuran



2,3,7,8-tetrachlorodibenzodioxin

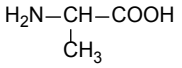
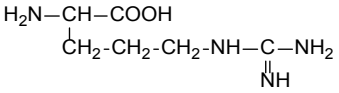
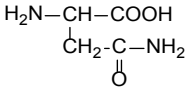
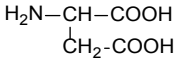
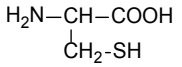
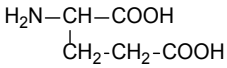
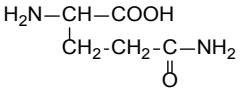
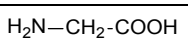
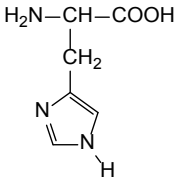
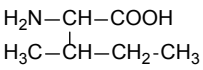
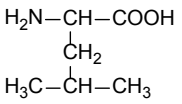


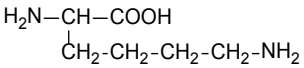
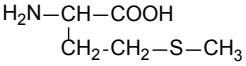
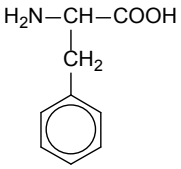
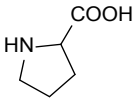
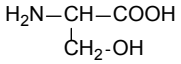
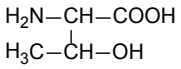
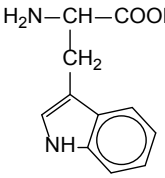
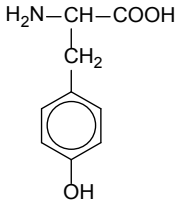
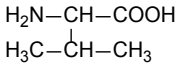
polychlorinated dibenzo-*p*-dioxin

32. Solubility product constants at 298 K

Compound	K_{sp}
$BaCO_3$	2.58×10^{-9}
$Ba(OH)_2 \cdot 8H_2O$	2.55×10^{-4}
$BaSO_4$	1.08×10^{-10}
$CdCO_3$	1.0×10^{-12}
$Cd(OH)_2$	7.2×10^{-15}
$PbCO_3$	7.40×10^{-14}
$Pb(OH)_2$	1.43×10^{-20}
$PbSO_4$	2.53×10^{-8}
Hg_2CO_3	3.6×10^{-17}
Hg_2SO_4	6.5×10^{-7}
$NiCO_3$	1.42×10^{-7}
$Ni(OH)_2$	5.48×10^{-16}
Ag_2CO_3	8.46×10^{-12}
Ag_2SO_4	1.20×10^{-5}
$ZnCO_3$	1.46×10^{-10}
$Zn(OH)_2$	3.0×10^{-17}

33. 2-amino acids

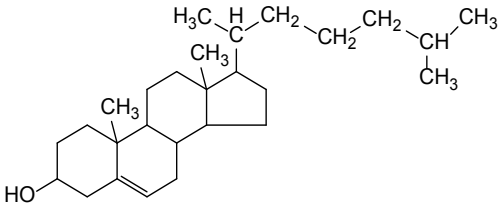
Common name	Symbol	Structural formula	pH of isoelectric point
alanine	Ala		6.0
arginine	Arg		10.8
asparagine	Asn		5.4
aspartic acid	Asp		2.8
cysteine	Cys		5.1
glutamic acid	Glu		3.2
glutamine	Gln		5.7
glycine	Gly		6.0
histidine	His		7.6
isoleucine	Ile		6.0
leucine	Leu		6.0

Common name	Symbol	Structural formula	pH of isoelectric point
lysine	Lys		9.7
methionine	Met		5.7
phenylalanine	Phe		5.5
proline	Pro		6.3
serine	Ser		5.7
threonine	Thr		5.6
tryptophan	Trp		5.9
tyrosine	Tyr		5.7
valine	Val		6.0

34. Lipids, carbohydrates and nucleotide components

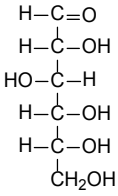
Lipids

Octanoic acid	$CH_3(CH_2)_6COOH$
Lauric acid	$CH_3(CH_2)_{10}COOH$
Palmitic acid	$CH_3(CH_2)_{14}COOH$
Stearic acid	$CH_3(CH_2)_{16}COOH$
Oleic acid	$CH_3(CH_2)_7CH{=}CH(CH_2)_7COOH$
Linoleic acid	$CH_3(CH_2)_4(CH{=}CHCH_2)_2(CH_2)_6COOH$
α-Linolenic acid	$CH_3CH_2(CH{=}CHCH_2)_3(CH_2)_6COOH$

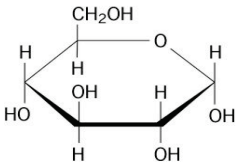


cholesterol

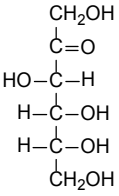
Carbohydrates



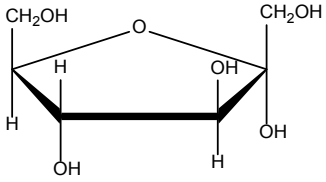
straight chain glucose



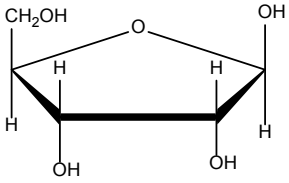
α-glucose



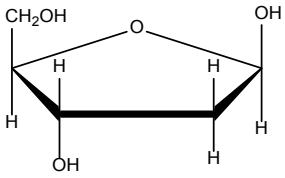
straight chain fructose



fructose

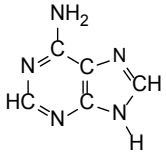


ribose

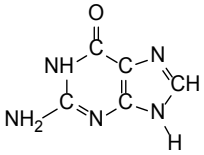


deoxyribose

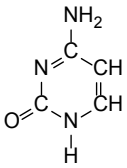
Nitrogenous bases



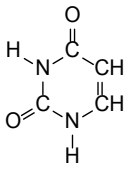
adenine



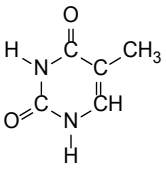
guanine



cytosine



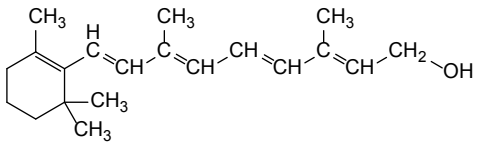
uracil



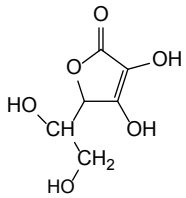
thymine

35. Vitamins and pigments

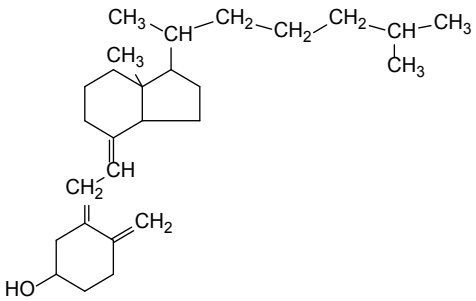
Vitamins



retinol (vitamin A)

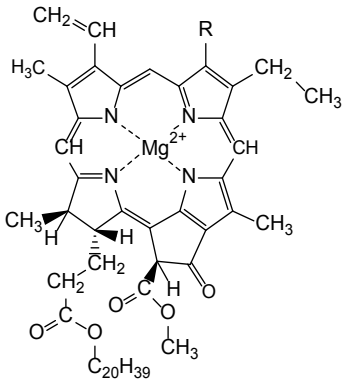


ascorbic acid (vitamin C)

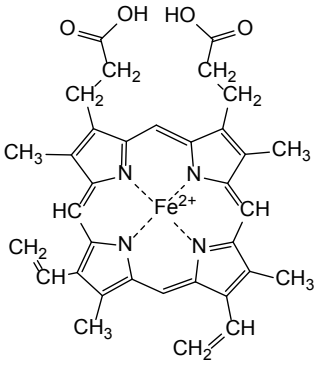


vitamin D (D3)

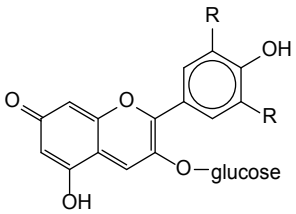
Pigments



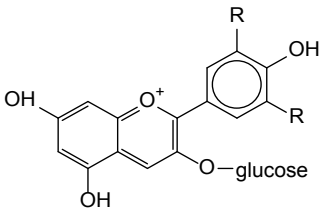
chlorophyll



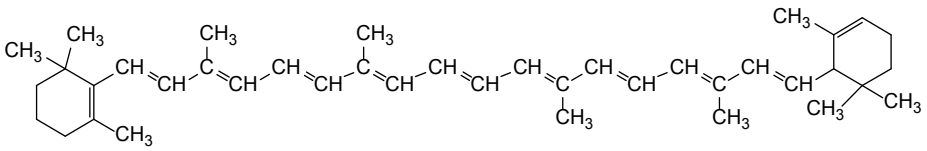
heme B



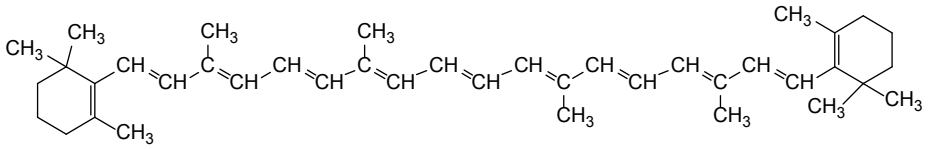
quinoidal base (blue)



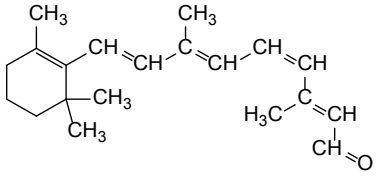
flavylium cation (red)



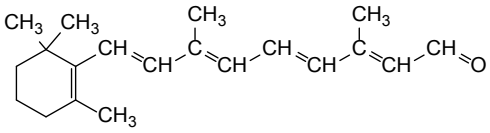
α-carotene



β-carotene

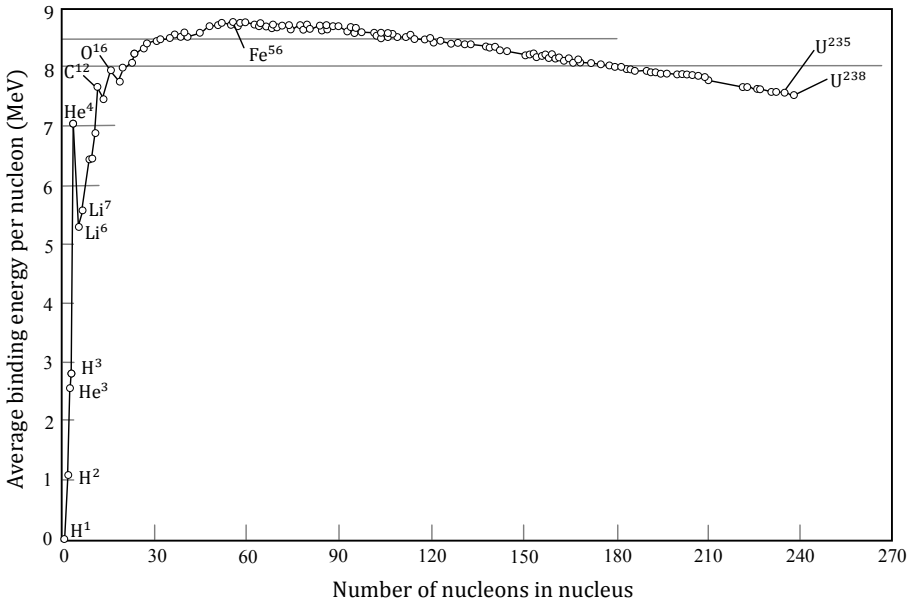


11-cis-*retinal*

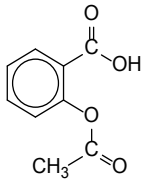


all-trans-*retinal*

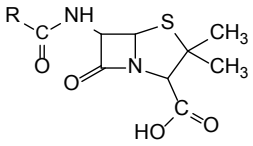
36. Binding energy curve



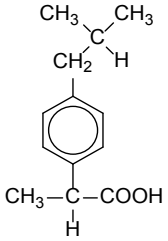
37. Representations of some medicinal molecules



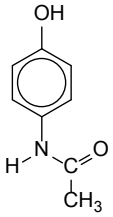
aspirin



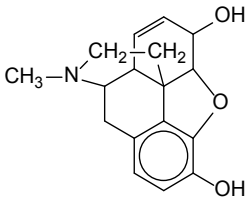
penicillin (general structure)



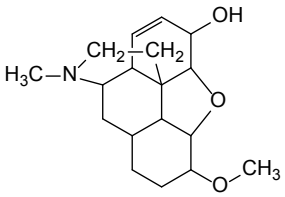
ibuprofen



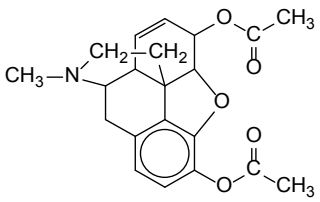
paracetamol (acetaminophen)



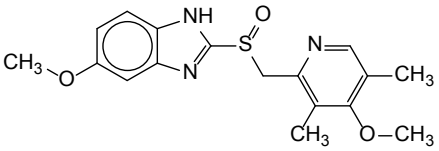
morphine



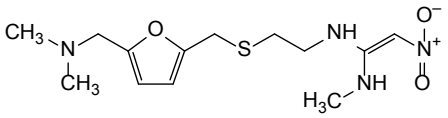
codeine



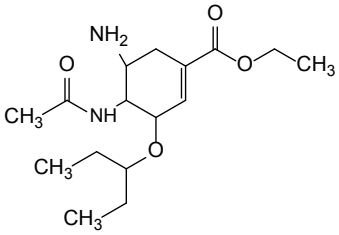
diamorphine (heroin)



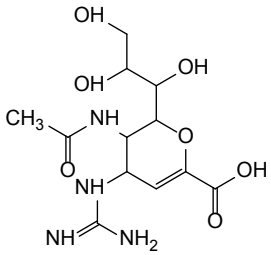
omeprazole



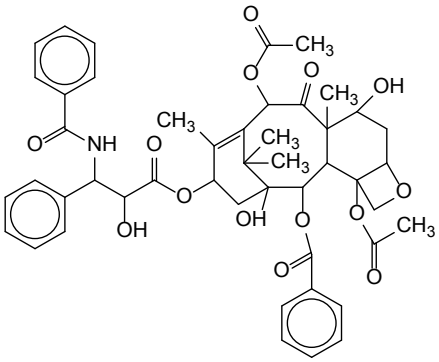
ranitidine



oseltamivir



zanamivir



taxol

38. References

Data in sections 9, 10, 11, 12, 13, 22, 26 and 27 was taken fully or in part from:

Aylward, G and Findlay, T. 2008. *SI chemical data*. (5th edition). Queensland, Australia. John Wiley & Sons.

Data in section 20 reproduced by permission of The Royal Society of Chemistry.

Barret, J. 2003. *Inorganic chemistry in aqueous solution*. London, UK. Royal Society of Chemistry.

Data in section 13 was taken in part from:

Burgess, DR. 2012. "Thermochemical Data". *NIST Chemistry WebBook, NIST Standard Reference Database*. Number 69. http://webbook.nist.gov.

Data in sections 7, 8, 9, 12, 13, 18, 19, 21, 23, 24, 28, 32, 33 was taken fully or in part from:

Haynes, WM, (ed). 2012. *CRC Handbook of chemistry and physics*. (93rd edition). Boca Raton, US. CRC Press.

Data in section 29 can be found in the following source:

Leach, MR. 2013. *Timeline of structural theory*. 04 January 2013. http://www.meta-synthesis.com/webbook/30_timeline/timeline.html.