

# **Chemistry data booklet**

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# Diploma Programme Chemistry data booklet

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#### 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	$\Delta G^{\Theta} = \Delta H^{\Theta} - T \Delta S^{\Theta}$
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	$\Delta G^{\bullet} = -RT \ln K$
19.1	$\Delta G^{\Theta} = -nFE^{\Theta}$
A.5	% 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	Energy density $=$ $\frac{\text{energy released from fuel}}{\text{volume of fuel consumed}}$
C.1	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  $N_A$ ) =  $6.02 \times 10^{23} \text{ mol}^{-1}$ 

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

Molar volume of an ideal gas at STP =  $2.27~\times10^{-2}~\text{m}^3~\text{mol}^{-1} = 22.7~\text{dm}^3~\text{mol}^{-1}$ 

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

STP conditions = 273 K and 100 kPa

SATP conditions = 298 K and 100 kPa

Speed of light =  $3.00\times10^8~ms^{-1}$ 

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

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

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

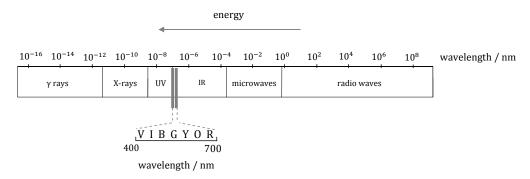
Ionic product constant for water  $(K_w) = 1.00 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$  at 298 K

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

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### 3. The electromagnetic spectrum



### 4. Fundamental particles

	Proton	Neutron	Electron
Mass (kg)	$1.672622 \times 10^{-27}$	$1.674927 \times 10^{-27}$	$9.109383 \times 10^{-31}$
Charge (C)	$1.602189 \times 10^{-19}$	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	Ва	56
berkelium	Bk	97
beryllium	Be	4
bismuth	Bi	83
bohrium	Bh	107
boron	В	5
bromine	Br	35
cadmium	Cd	48
caesium	Cs	55
calcium	Ca	20
californium	Cf	98
carbon	С	6
cerium	Ce	58
chlorine	Cl	17
chromium	Cr	24
cobalt	Со	27
copernicium	Cn	112
copper	Cu	29
curium	Cm	96
darmstadtium	Ds	110
dubnium	Db	105
I		

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	Не	2
holmium	Но	67
hydrogen	Н	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	0	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	Та	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

232.04

231.04

238.03

(237)

(244)

(243)

(247)

(251)

(247)

(252)

(257)

(258)

(262)



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

-259.2						Melting p	ooint (°C)										
H																	He
-252.9		_				Elen	nent										-268.9
180.5	1287											2077	3500	-210.0	-218.8	-219.7	-248.6
Li	Be					Boiling p	oint (°C)					В	С	N	0	F	Ne
1342	2468											4000	4827	-195.8	-183.0	-188.1	-246.0
97.79	650.0											660.3	1414	44.15	115.2	-101.5	-189.3
Na	Mg											Al	Si	P	S	Cl	Ar
882.9	1090											2519	3265	280.5	444.6	-34.04	-185.8
63.38	842.0	1541	1670	1910	1907	1246	1538	1495	1455	1085	419.5	29.77	938.2	816.8	220.8	-7.050	-157.4
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
758.8	1484	2836	3287	3407	2671	2061	2861	2927	2913	2560	907.0	2229	2833	613.0	684.8	58.78	-153.4
39.30	768.8	1522	1854	2477	2622	2157	2333	1963	1555	961.8	321.1	156.6	231.9	630.6	449.5	113.7	-111.8
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те	I	Xe
687.8	1377	3345	4406	4741	4639	4262	4147	3695	2963	2162	766.8	2027	2586	1587	987.8	184.4	-108.1
28.44	725.0	920.0	2233	3017	3414	3453	3033	2446	1768	1064	-38.83	303.8	327.5	271.4	253.8	301.8	-71.15
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
670.8	1845	3464	4600	5455	5555	5900	5008	4428	3825	2836	356.6	1473	1749	1564	962.0	336.8	-61.85
27.00	699.8	1050															
Fr	Ra	Ac															
676.8	1140	3200															

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

1312 <b>–</b> 73 <b>H</b> 2.2			First ionization Electron affinity (kJ mol <sup>-1</sup> ) energy (kJ mol <sup>-1</sup> ) (2nd EA / kJ mol <sup>-1</sup> )													2372 <b>He</b>	
520 <b>–</b> 60	900					Element						801 -27	1086 -122	1402	1314 -141 (+753)	1681 -328	2081
Li	Ве											В	С	N	0	F	Ne
1.0	1.6				Ele	ctronegativ	vity					2.0	2.6	3.0	3.4	4.0	
496 <b>–</b> 53	738											578 -42	787 -134	1012 -72	1000 -200 (+545)	1251 -349	1520
Na	Mg											Al	Si	P	S	Cl	Ar
0.9	1.3											1.6	1.9	2.2	2.6	3.2	
419 -48	590 –2	633 -18	659 -8	651 -51	653 -64	717	762 -15	760 -64	737 -112	745 -119	906	579 -41	762 -119	944 -78	941 -195	1140 -325	1351
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
8.0	1.0	1.4	1.5	1.6	1.7	1.6	1.8	1.9	1.9	1.9	1.6	1.8	2.0	2.2	2.6	3.0	
403 <b>-</b> 47	549 -5	600 -30	640 -41	652 -88	684 -72	702 -53	710 -101	720 -110	804 -54	731 -126	868	558 –29	709 -107	831 -101	869 -190	1008 -295	1170
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Хe
0.8				110	1-10	10				4-1-		111		00			
	1.0	1.2	1.3	1.6	2.2	2.1	2.2	2.3	2.2	1.9	1.7	1.8	2.0	2.0	2.1	2.7	2.6
376 -46	1.0 503 -14															2.7	2.6
376 –46 <b>Cs</b>	_	1.2	1.3	1.6	2.2	2.1	2.2	2.3	2.2	1.9	1.7	1.8	2.0	2.0	2.1		
	503 -14	1.2 538 –45	1.3 659 –1	1.6 728 –31	2.2 759 –79	2.1 756 –14	2.2 814 -106	2.3 865 –151	2.2 864 –205	1.9 890 –223	1.7	1.8 589 -36	2.0 716 -35	2.0 703 –91	2.1 812 –183	-270	1037
Cs	503 -14 <b>Ba</b>	1.2 538 -45 <b>La</b>	1.3 659 -1 <b>Hf</b>	1.6 728 -31 <b>Ta</b>	2.2 759 –79	2.1 756 –14 <b>Re</b>	2.2 814 -106 <b>Os</b>	2.3 865 –151 <b>Ir</b>	2.2 864 -205 <b>Pt</b>	1.9 890 –223 <b>Au</b>	1.7 1007 <b>Hg</b>	1.8 589 -36 <b>Tl</b>	2.0 716 -35 <b>Pb</b>	2.0 703 -91 <b>Bi</b>	2.1 812 -183 <b>Po</b>	-270 <b>At</b>	1037





# 9. Atomic and ionic radii of the elements

32 <b>H</b>						(10-	radius <sup>12</sup> m)										37 <b>He</b>
130 <b>Li</b> 76 (1+)	99 <b>Be</b> 45 (2+)					Ionic	nent radius <sup>12</sup> m)					84 <b>B</b> 27 (3+)	75 <b>C</b> 16 (4+)	71 <b>N</b> 146 (3-)	64 <b>0</b> 140 (2-)	60 <b>F</b> 133 (1-)	62 <b>Ne</b>
160 <b>Na</b> 102 (1+)	140 <b>Mg</b> 72 (2+)											124 <b>Al</b> 54 (3+)	114 <b>Si</b> 40 (4+)	109 <b>P</b> 38 (5+)	104 <b>S</b> 184 (2-)	100 <b>Cl</b> 181 (1–)	101 <b>Ar</b>
200 <b>K</b> 138 (1+)	174 <b>Ca</b> 100 (2+)	159 <b>Sc</b> 75 (3+)	148 <b>Ti</b> 86 (2+) 61 (4+)	144 <b>V</b> 79 (2+) 54 (5+)	130 <b>Cr</b> 62 (3+) 44 (6+)	129 <b>Mn</b> 83 (2+) 53 (4+)	124 <b>Fe</b> 61 (2+) 55 (3+)	118 <b>Co</b> 65(+2) 55 (+3)	117 <b>Ni</b> 69 (2+)	122 <b>Cu</b> 77 (1+) 73 (2+)	120 <b>Zn</b> 74 (2+)	123 <b>Ga</b> 62(3+)	120 <b>Ge</b> 53 (4+) 272(4-)	120 <b>As</b> 58 (3+) 46 (5+)	118 <b>Se</b> 198 (2-)	117 <b>Br</b> 196 (1–)	116 <b>Kr</b>
215 <b>Rb</b> 152 (1+)	190 <b>Sr</b> 118 (2+)	176 <b>Y</b> 90 (3+)	164 <b>Zr</b> 72 (4+)	156 <b>Nb</b> 72 (3+) 64 (5+)	146 <b>Mo</b> 65 (4+)	138 <b>Tc</b> 65(4+)	136 <b>Ru</b> 68(3+) 62 (4+)	134 <b>Rh</b> 67 (+3) 60 (+4)	130 <b>Pd</b> 86(2+) 62(4+)	136 <b>Ag</b> 115 (1+)	140 <b>Cd</b> 95 (2+)	142 <b>In</b> 80(3+)	140 <b>Sn</b> 118(2+) 69 (4+)	140 <b>Sb</b> 76 (3+)	137 <b>Te</b> 221 (2-)	136 <b>I</b> 220(1-)	136 <b>Xe</b>
238 <b>Cs</b> 167 (1+)	206 <b>Ba</b> 135 (2+)	194 <b>La</b> 103 (3+)	164 <b>Hf</b> 71 (4+)	158 <b>Ta</b> 64 (5+)	150 <b>W</b> 66 (4+) 60(6+)	141 <b>Re</b> 63(4+) 53(7+)	136 <b>Os</b> 63 (4+) 55(6+)	132 <b>Ir</b> 68(+3) 63 (+4)	130 <b>Pt</b> 80(2+) 63(4+)	130 <b>Au</b> 137 (1+) 85 (3+)	132 <b>Hg</b> 119 (1+) 102 (2+)	144 <b>Tl</b> 150 (1+) 89 (3)	145 <b>Pb</b> 119 (2+) 78 (4+)	150 <b>Bi</b> 103 (3+) 76(5+)	142 <b>Po</b> 97(4+)	148 <b>At</b>	146 <b>Rn</b>
242 <b>Fr</b>	211 <b>Ra</b>	201 <b>Ac</b>															

# 10. Covalent bond lengths

### Single bonds $(10^{-12} \text{m} = \text{pm})$

	Br	С	Cl	F	Н	I	N	0	P	S	Si
Br	228	194	214	176	141	247	214		220	227	216
С	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
Н	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
0		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	$N \equiv N$	110
C≡C	120	C=0 122	N=O	114
C=C (in benzene)	140	C=S 156	0=0	121
C=N	130	N=N 125	S=S	189

## 11. Bond enthalpies and average bond enthalpies at 298 $\ensuremath{\mathrm{K}}$

## Single bonds (kJ $mol^{-1}$ )

	Br	С	Cl	F	Н	I	N	0	P	S	Si
Br	193	285	219	249	366	178		201	264	218	330
С	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
Н	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			
0	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	$N \equiv N$	945
C≡C	839	C=O	804	N=O	587
C=C (in benzene)	507	C=S	536	0=0	498
C=N	615	N=N	470	S=S	429

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# 12. Selected compounds—thermodynamic data

Substance	Formula	State	$\Delta H_{\rm f}^{\oplus} ({\rm kJ\ mol^{-1}})$	$\Delta G_{\rm f}^{\rm e}  ({ m kJ  mol^{-1}})$	$S^{\Theta}(J \text{ K}^{-1} \text{ mol}^{-1})$
methane	CH <sub>4</sub>	g	-74.0	-50.0	+186
ethane	$C_2H_6$	g	-84.0	-32.0	+230
propane	C <sub>3</sub> H <sub>8</sub>	g	-105	-24.0	+270
butane	$C_4H_{10}$	g	-126	-17.0	+310
pentane	C <sub>5</sub> H <sub>12</sub>	ĺ	-173		
hexane	C <sub>6</sub> H <sub>14</sub>	1	-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 <sub>4</sub> H <sub>8</sub>	g	+0.10	+71.0	+306
<i>cis</i> -but-2-ene	C <sub>4</sub> H <sub>8</sub>	g	-7.0	+66.0	+301
trans-but-2-ene	C <sub>4</sub> H <sub>8</sub>	g	-11.0	+63.0	+297
ethyne	$C_2H_2$	g	+228	+211	+201
propyne	C <sub>3</sub> H <sub>4</sub>	g	+185	+194	+248
buta-1,3-diene	C <sub>4</sub> H <sub>6</sub>	g	+110	+151	+279
cvclohexane	$C_{6}H_{12}$	l	-156	1131	1277
benzene	C <sub>6</sub> H <sub>12</sub>	1	+49.0	+125	+173
methylbenzene	$C_6H_5CH_3$	1	+12.0	T123	T1/3
ethylbenzene	$C_6H_5CH_2CH_3$	1	-12.0 -12.0		
phenylethene	$C_6H_5CH_2CH_3$	1	-12.0 + 104		
chloromethane	CH <sub>3</sub> Cl	_	-82.0	-58.0	+235
dichloromethane		g l	-62.0 -124	-36.0	
trichloromethane	CH <sub>2</sub> Cl <sub>2</sub>	1	-124 -134	-74.0	+178 +202
	CHCl <sub>3</sub>				
bromomethane	CH₃Br	g l	-36.0	-26.0	+246
iodomethane	CH <sub>3</sub> I	_	-14.0	F0.0	+163
chloroethane	C <sub>2</sub> H <sub>5</sub> Cl	g	-137	-53.0	. 400
bromoethane	C <sub>2</sub> H <sub>5</sub> Br	1	-90.0	-26.0	+199
chlorobenzene	C <sub>6</sub> H <sub>5</sub> Cl	1	+11.0	4.65	. 405
methanol	CH <sub>3</sub> OH	l	-239	-167	+127
ethanol	C <sub>2</sub> H <sub>5</sub> OH	l	-278	-175	+161
phenol	C <sub>6</sub> H <sub>5</sub> OH	S	-165		+144
methanal	НСНО	g	-109	-102	+219
ethanal	CH <sub>3</sub> CHO	g	-166	-133	+264
propanone	$(CH_3)_2CO$	l	-248		+200
methanoic acid	НСООН	l	-425	-361	+129
ethanoic acid	CH <sub>3</sub> COOH	l	-484	-390	+160
benzoic acid	C <sub>6</sub> H <sub>5</sub> COOH	S	-385		+168
methylamine	CH <sub>3</sub> NH <sub>2</sub>	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 <sub>2</sub>	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
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# 13. Enthalpies of combustion

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

Substance	Formula	State	$\Delta H_{\rm c}^{\rm e}$ (kJ mol <sup>-1</sup> )
hydrogen	$H_2$	g	-286
sulfur	S	s	-297
carbon (graphite)	С	S	-394
carbon monoxide	CO	g	-283
methane	CH <sub>4</sub>	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 <sub>2</sub> H <sub>5</sub> Cl	g	-1413
iodoethane	$C_2H_5I$	l	-1463
trichloromethane	CHCl <sub>3</sub>	l	-473
methanol	CH <sub>3</sub> OH	l	-726
ethanol	C <sub>2</sub> H <sub>5</sub> OH	l	-1367

Substance	Formula	State	$\Delta H_{\rm c}^{\oplus}$ (kJ mol <sup>-1</sup> )
propan-1-ol	C <sub>3</sub> H <sub>7</sub> OH	1	-2021
butan-1-ol	$C_4H_9OH$	1	-2676
cyclohexanol	C <sub>6</sub> H <sub>11</sub> OH	S	-3728
phenol	C <sub>6</sub> H <sub>5</sub> OH	S	-3053
ethoxyethane	$(C_2H_5)_2O$	1	-2724
methanal	НСНО	g	-571
ethanal	CH <sub>3</sub> CHO	g	-1167
benzaldehyde	C <sub>6</sub> H <sub>5</sub> CHO	l	-3525
propanone	$(CH_3)_2CO$	l	-1790
pentan-3-one	$(C_2H_5)_2CO$	l	-3100
phenylethanone	CH <sub>3</sub> COC <sub>6</sub> H <sub>5</sub>	l	-4149
methanoic acid	НСООН	l	-255
ethanoic acid	CH <sub>3</sub> COOH	l	-874
benzoic acid	C <sub>6</sub> H <sub>5</sub> COOH	S	-3228
ethanedioic acid	$(COOH)_2$	S	-243
ethyl ethanoate	$CH_3COOC_2H_5$	l	-2238
ethanamide	CH <sub>3</sub> CONH <sub>2</sub>	S	-1186
methylamine	CH <sub>3</sub> NH <sub>2</sub>	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					

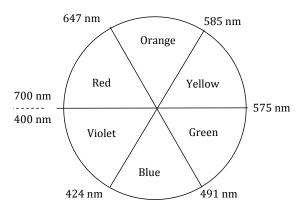
## 15. Spectrochemical series

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

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

## 16. Ligands

### 17. Colour wheel



### 18. Lattice enthalpies at 298 K (experimental values)

The lattice enthalpy values  $(\Delta H^e_{lattice})$  given relate to the endothermic process  $M_a X_b(s) \to a M^{b+}(g) + b X^{a-}(g)$  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	$\Delta H_{ m lattice}^{ m e} ({ m kJ mol}^{-1})$							
	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	$\Delta H_{\text{lattice}}^{\Theta} (kJ \text{ mol}^{-1})$
CaF <sub>2</sub>	2651
BeCl <sub>2</sub>	3033
${ m MgCl}_2$	2540
CaCl <sub>2</sub>	2271
SrCl <sub>2</sub>	2170
BaCl <sub>2</sub>	2069
MgO	3791
CaO	3401

Other substances	$\Delta H_{\text{lattice}}^{\Theta} (\mathbf{kJ}  \mathbf{mol^{-1}})$
SrO	3223
BaO	3054
CuCl <sub>2</sub>	2824
AgF	974
AgCl	918
AgBr	905
AgI	892

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# 19. Enthalpies of aqueous solutions

Solute	$\Delta H_{\rm sol}^{\rm e}$ (kJ mol <sup>-1</sup> )
NH <sub>4</sub> Cl	+14.78
$\mathrm{NH_4NO_3}$	+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
NaF NaCl NaBr NaI	+0.91 +3.88 -0.60 -7.53

Solute	$\Delta H_{\rm sol}^{\Theta}$ (kJ mol <sup>-1</sup> )
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	$\Delta H_{\mathrm{hyd}}^{\mathrm{e}}$ (kJ mol <sup>-1</sup> )
Li <sup>+</sup>	-538
Na <sup>+</sup>	-424
K <sup>+</sup>	-340
Rb <sup>+</sup>	-315
Cs <sup>+</sup>	-291
Be <sup>2+</sup>	-2524
Mg <sup>2+</sup>	-1963
Ca <sup>2+</sup>	-1616
Sr <sup>2+</sup>	-1483
Ba <sup>2+</sup>	-1346
Ra <sup>2+</sup>	-1335
Al <sup>3+</sup>	-4741
Ga <sup>3+</sup>	-4745
In <sup>3+</sup>	-4171
Tl <sup>3+</sup>	-4163
Tl <sup>+</sup>	-346
Sn <sup>2+</sup>	-1587
Pb <sup>2+</sup>	-1523
I	

Anions	$\Delta H_{\mathrm{hyd}}^{\mathrm{e}}$ (kJ mol <sup>-1</sup> )
F-	-504
Cl-	-359
Br <sup>-</sup>	-328
I-	-287
ClO <sub>3</sub>	-331
BrO <sub>3</sub>	-358
IO <sub>3</sub>	-446
ClO <sub>4</sub>	-205
OH-	-519
CN-	-341
NO <sub>3</sub>	-316
HCO <sub>3</sub>	-383
CO <sub>3</sub> <sup>2-</sup>	-1486
HSO <sub>4</sub>	-362
SO <sub>4</sub> <sup>2-</sup>	-1099
PO <sub>4</sub> <sup>3-</sup>	-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  $pK_b$ 

#### Carboxylic acids

Name	Formula	pK <sub>a</sub>
methanoic	НСООН	3.75
ethanoic	CH <sub>3</sub> COOH	4.76
propanoic	CH <sub>3</sub> CH <sub>2</sub> COOH	4.87
butanoic	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> COOH	4.83
2-methylpropanoic	(CH <sub>3</sub> ) <sub>2</sub> CHCOOH	4.84
pentanoic	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> COOH	4.83
2,2-dimethylpropanoic	(CH <sub>3</sub> ) <sub>3</sub> CCOOH	5.03
benzoic	C <sub>6</sub> H <sub>5</sub> COOH	4.20
phenylethanoic	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> COOH	4.31

#### Halogenated carboxylic acids

Name	Formula	pK <sub>a</sub>
chloroethanoic	CH₂ClCOOH	2.87
dichloroethanoic	CHCl <sub>2</sub> COOH	1.35
trichloroethanoic	CCl₃COOH	0.66
fluoroethanoic	CH <sub>2</sub> FCOOH	2.59
bromoethanoic	CH <sub>2</sub> BrCOOH	2.90
iodoethanoic	CH <sub>2</sub> ICOOH	3.18

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#### Phenols

Name	Formula	pK <sub>a</sub>
phenol	C <sub>6</sub> H <sub>5</sub> OH	9.99
2-nitrophenol	O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> OH	7.23
3-nitrophenol	O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> OH	8.36
4-nitrophenol	O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> OH	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 <sub>a</sub>
methanol	CH <sub>3</sub> OH	15.5
ethanol	$C_2H_5OH$	15.5

#### Amines

Name	Formula	pK <sub>b</sub>
ammonia	NH <sub>3</sub>	4.75
methylamine	CH <sub>3</sub> NH <sub>2</sub>	3.34
ethylamine	CH <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>	3.35
dimethylamine	(CH <sub>3</sub> ) <sub>2</sub> NH	3.27
trimethylamine	$(CH_3)_3N$	4.20
diethylamine	$(C_2H_5)_2NH$	3.16
triethylamine	$(C_2H_5)_3N$	3.25
phenylamine	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	9.13

#### 22. Acid-base indicators

		Colour change		
Indicator	pK <sub>a</sub>	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 <sub>w</sub> value
0	$0.113 \times 10^{-14}$
5	$0.185 \times 10^{-14}$
10	$0.292 \times 10^{-14}$
15	$0.453 \times 10^{-14}$
20	$0.684 \times 10^{-14}$
25	$1.00 \times 10^{-14}$
30	$1.47 \times 10^{-14}$
35	$2.09 \times 10^{-14}$
40	$2.92 \times 10^{-14}$
45	$4.02 \times 10^{-14}$
50	$5.43 \times 10^{-14}$
55	$7.24 \times 10^{-14}$
60	$9.55 \times 10^{-14}$
65	$12.4 \times 10^{-14}$
70	$15.9 \times 10^{-14}$
75	$20.1 \times 10^{-14}$
80	$25.2 \times 10^{-14}$
85	$31.3 \times 10^{-14}$
90	$38.3 \times 10^{-14}$
95	$46.6 \times 10^{-14}$
100	$56.0 \times 10^{-14}$

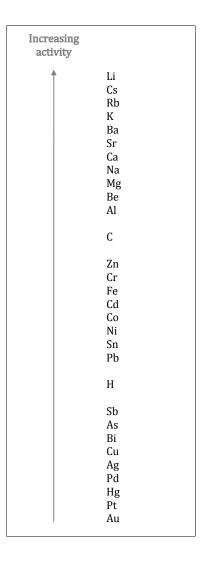


# 24. Standard electrode potentials at 298 K

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

Oxidized species	-	Reduced species	$E^{\Theta}(V)$
$Cu^{2+}(aq) + e^{-}$		Cu <sup>+</sup> (aq)	+0.15
$SO_4^{2-}(aq) + 4H^+(aq) + 2e^-$		$\mathrm{H_2SO_3(aq)} + \mathrm{H_2O(l)}$	+0.17
$Cu^{2+}(aq) + 2e^{-}$	<del></del>	Cu(s)	+0.34
$\frac{1}{2}O_2(g) + H_2O(l) + 2e^-$		20H <sup>-</sup> (aq)	+0.40
Cu <sup>+</sup> (aq) + e <sup>-</sup>		Cu(s)	+0.52
$\frac{1}{2}I_2(s) + e^-$		I <sup>-</sup> (aq)	+0.54
$Fe^{3+}(aq) + e^{-}$		Fe <sup>2+</sup> (aq)	+0.77
$Ag^{+}(aq) + e^{-}$	<del></del>	Ag(s)	+0.80
$\frac{1}{2}\mathrm{Br}_2(\mathrm{l}) + \mathrm{e}^-$	<del></del>	Br <sup>-</sup> (aq)	+1.09
$\frac{1}{2}O_2(g) + 2H_2(aq) + 2e^-$	<del></del>	H <sub>2</sub> O(l)	+1.23
$Cr_2O_7^{2-}(aq) + 14H^+(aq) + 6e^-$		$2Cr^{3+}(aq) + 7H_2O(l)$	+1.36
$\frac{1}{2}\operatorname{Cl}_{2}(g) + e^{-}$	<del></del>	Cl <sup>-</sup> (aq)	+1.36
$MnO_4^-(aq) + 8H^+(aq) + 5e^-$	<del></del>	$Mn^{2+} + 4H_2O(l)$	+1.51
$\frac{1}{2}F_2(g) + e^-$	-	F <sup>-</sup> (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 <sup>-1</sup> )		Intensity	
C-I	iodoalkanes	490-620	strong	
C-Br	bromoalkanes	500-600	strong	
C-Cl	chloroalkanes	600-800	strong	
C-F	fluoroalkanes 1000–1400 st		strong	
C-O	alcohols, esters, ethers	1050-1410	strong	
C=C	alkenes	1620-1680	medium-weak; multiple bands	
C=0	aldehydes, ketones, carboxylic acids and esters	1700-1750	strong	
C≡C	alkynes	2100-2260	variable	
О-Н	hydrogen bonding in carboxylic acids	onding in carboxylic acids 2500–3000 strong, very broading in carboxylic acids		
С–Н	alkanes, alkenes, arenes 2850–3090		strong	
О-Н	hydrogen bonding in alcohols and phenols 3200–3600 strong, broa		strong, broad	
N-H	primary amines 3300–3500 mediu		medium, two bands	

## 27. <sup>1</sup>H NMR data

### Typical proton chemical shift values (\delta) 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 <b>H</b> <sub>3</sub>	0.9-1.0
—C <b>H</b> <sub>2</sub> -R	1.3-1.4
—R <sub>2</sub> C <b>H</b>	1.5
O ROCH <sub>2</sub> —	2.0-2.5
R CH <sub>2</sub> —	2.2-2.7
—————————————————————————————————————	2.5-3.5
—C≡C− <b>H</b>	1.8-3.1
—C <b>H</b> <sub>2</sub> -Hal	3.5-4.4
R-O-CH <sub>2</sub> -	3.3-3.7
O R O CH <sub>2</sub> —	3.7-4.8
O R / C \ O – <b>H</b>	9.0–13.0
R-O- <b>H</b>	1.0-6.0
HC=C <b>H</b> <sub>2</sub>	4.5-6.0

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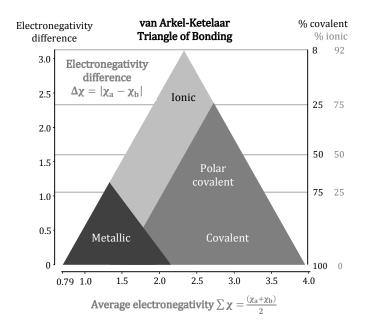


Type of proton	Chemical shift (ppm)
————ОН	4.0–12.0
————	6.9–9.0
O R ~ H	9.4–10.0

# 28. Mass spectral fragments lost

Mass lost	Fragment lost	
15	CH <sub>3</sub>	
17	ОН	
18	H <sub>2</sub> O	
28	$CH_2=CH_2$ , $C=0$	
29	CH <sub>3</sub> CH <sub>2</sub> , CHO	
31	CH <sub>3</sub> O	
45	СООН	

### 29. Triangular bonding diagram



#### 30. Resin identification codes

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

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

# 31. Representations of some materials molecules

$$CI_m$$

polychlorinated biphenyls

$$\binom{0}{0}$$

1,4-dioxin

$$CI_n$$
  $CI_m$ 

polychlorinated dibenzofuran

2,3,7,8-tetrachlorodibenzodioxin

$$CI_{n}$$
  $CI_{m}$ 

polychlorinated dibenzo-p-dioxin

# 32. Solubility product constants at 298 $\ensuremath{\mathrm{K}}$

Compound	$K_{\mathrm{sp}}$
BaCO <sub>3</sub>	$2.58 \times 10^{-9}$
Ba(OH) <sub>2</sub> · 8H <sub>2</sub> O	$2.55 \times 10^{-4}$
BaSO <sub>4</sub>	$1.08 \times 10^{-10}$
CdCO <sub>3</sub>	$1.0 \times 10^{-12}$
Cd(OH) <sub>2</sub>	$7.2 \times 10^{-15}$
PbCO <sub>3</sub>	$7.40 \times 10^{-14}$
Pb(OH) <sub>2</sub>	$1.43 \times 10^{-20}$
PbSO <sub>4</sub>	$2.53 \times 10^{-8}$
Hg <sub>2</sub> CO <sub>3</sub>	$3.6 \times 10^{-17}$
Hg <sub>2</sub> SO <sub>4</sub>	$6.5 \times 10^{-7}$
NiCO <sub>3</sub>	$1.42 \times 10^{-7}$
Ni(OH) <sub>2</sub>	$5.48 \times 10^{-16}$
$Ag_2CO_3$	$8.46 \times 10^{-12}$
Ag <sub>2</sub> SO <sub>4</sub>	$1.20 \times 10^{-5}$
ZnCO <sub>3</sub>	$1.46 \times 10^{-10}$
Zn(OH) <sub>2</sub>	$3.0 \times 10^{-17}$

#### 33. 2-amino acids

Common name	Symbol	Structural formula	pH of isoelectric point
alanine	Ala	H₂N−CH−COOH CH₃	6.0
arginine	Arg	H <sub>2</sub> N—CH—COOH CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -NH—C—NH <sub>2</sub> NH	10.8
asparagine	Asn	H <sub>2</sub> N-CH-COOH CH <sub>2</sub> -C-NH <sub>2</sub> Ö	5.4
aspartic acid	Asp	H₂N−CH−COOH CH₂-COOH	2.8
cysteine	Cys	H <sub>2</sub> N—CH—COOH CH <sub>2</sub> -SH	5.1
glutamic acid	Glu	H <sub>2</sub> N—CH—COOH CH <sub>2</sub> -CH <sub>2</sub> -COOH	3.2
glutamine	Gln	H <sub>2</sub> N-CH-COOH CH <sub>2</sub> -CH <sub>2</sub> -C-NH <sub>2</sub> O	5.7
glycine	Gly	H <sub>2</sub> N-CH <sub>2</sub> -COOH	6.0
histidine	His	H <sub>2</sub> N-CH-COOH CH <sub>2</sub> N N H	7.6
isoleucine	Ile	H <sub>2</sub> N—CH—COOH H <sub>3</sub> C—CH—CH <sub>2</sub> -CH <sub>3</sub>	6.0
leucine	Leu	H₂N−CH−COOH cH₂ H₃C−cH−CH₃	6.0

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Common name	Symbol	Structural formula	pH of isoelectric point
lysine	Lys	H <sub>2</sub> N—CH—COOH CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -NH <sub>2</sub>	9.7
methionine	Met	H <sub>2</sub> N-CH-COOH CH <sub>2</sub> -CH <sub>2</sub> -S-CH <sub>3</sub>	5.7
phenylalanine	Phe	H <sub>2</sub> N-CH-COOH CH <sub>2</sub>	5.5
proline	Pro	COOH	6.3
serine	Ser	H <sub>2</sub> N-CH-COOH CH <sub>2</sub> -OH	5.7
threonine	Thr	H₂N−CH−COOH H₃C−CH−OH	5.6
tryptophan	Trp	H <sub>2</sub> N-CH-COOH CH <sub>2</sub>	5.9
tyrosine	Tyr	H <sub>2</sub> N-CH-COOH CH <sub>2</sub>	5.7
valine	Val	H₂N−CH−COOH H₃C−ĊH−CH₃	6.0

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### 34. Lipids, carbohydrates and nucleotide components

#### Lipids

Octanoic acid  ${\rm CH_3(CH_2)_6C00H}$  Lauric acid  ${\rm CH_3(CH_2)_{10}C00H}$  Palmitic acid  ${\rm CH_3(CH_2)_{14}C00H}$  Stearic acid  ${\rm CH_3(CH_2)_{16}C00H}$ 

Oleic acid  $CH_3(CH_2)_7CH=CH(CH_2)_7COOH$ 

Linoleic acid  $CH_3(CH_2)_4(CH=CHCH_2)_2(CH_2)_6COOH$ 

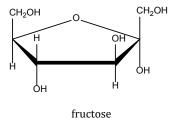
α-Linolenic acid  $CH_3CH_2(CH=CHCH_2)_3(CH_2)_6COOH$ 

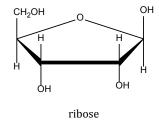
cholesterol

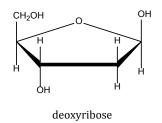
#### Carbohydrates

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#### Nitrogenous bases



adenine

guanine

$$\begin{array}{c} NH_2 \\ N \stackrel{C}{=} CH \\ O \stackrel{C}{=} N \stackrel{C}{=} CH \end{array}$$

uracil

thymine

### 35. Vitamins and pigments

#### Vitamins

$$\begin{array}{c} CH_3 & CH_3 & CH_3 \\ CCH_2 & CH_2 & CH_2 \\ CCH_3 & CH_2 & CH_2 \\ CCH_3 & CH_2 & CH_2 \\ CCH_3 & CH_2 & CH_2 & CH_2 \\ CCH_3 & CH_2 & CH_2 & CH_2 \\ CCH_3 & CH_2 & CH_2 & CH_2 \\ CCH_3 & CH_3 & CH_3 \\ CCH_3 & CH_2 & CH_2 & CH_2 \\ CCH_3 & CH_3 & CH_3 \\ CCH_3 & CH_2 & CH_2 & CH_2 \\ CCH_3 & CH_3 & CH_3 \\ CCH_3 & CCH_2 & CH_2 & CH_2 \\ CCH_3 & CCH_2 & CCH_2 & CCH_2 \\ CCH_3 & CCH_2 &$$

vitamin D (D3)

#### **Pigments**

chlorophyll

heme B

quinoidal base (blue)

flavylium cation (red)

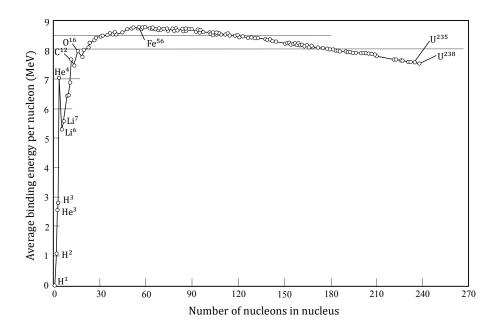
 $\alpha\text{-carotene}$ 

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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

$$H_3C-N$$
 $CH_2$ 
 $CH_2$ 
 $CH_2$ 
 $O$ 
 $CH_3$ 

codeine

$$\mathsf{CH}_3 - \mathsf{N} \underbrace{\mathsf{CH}_2 - \mathsf{CH}_2}_{\mathsf{C}} \underbrace{\mathsf{C}}_{\mathsf{C}} \underbrace{\mathsf{C}}_{\mathsf{C}}^{\mathsf{CH}_3}$$

diamorphine (heroin)

ome prazole

ranitidine

$$\begin{array}{c} O\\ O\\ C\\ C\\ H_3\\ C\\ H_3$$

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.

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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.

