

Chemistry data booklet First assessment 2016

Contents

1.	Some relevant equations	1
2.	Physical constants and unit conversions	2
3.	The electromagnetic spectrum	2
4.	Fundamental particles	2
5.	Names of the elements	3
6.	The periodic table	5
7.	Melting and boiling points of the elements	6
8.	First ionization energy, electron affinity and electronegativity of the elements	7
9.	Atomic and ionic radii of the elements	8
10.	Covalent bond lengths	9
11.	Bond enthalpies and average bond enthalpies at 298 K	10
12.	Selected compounds—thermodynamic data	11
13.	Enthalpies of combustion	13
14.	Common oxidation numbers of 3-D ions	14
15.	Spectrochemical series	14
16.	Ligands	14
17.	Colour wheel	15
18.	Lattice enthalpies at 298 K (experimental values)	15
19.	Enthalpies of aqueous solutions	16
20.	Enthalpies of hydration	16
21.	Strengths of organic acids and bases	17
22.	Acid-base indicators	18
23.	Ionization constant of water at varying temperatures	19
24.	Standard electrode potentials	20
25.	Activity series	21
26.	Infrared data	22
27.	¹ H NMR data	23
28.	Mass spectral fragments lost	24
29.	Triangular bonding diagram	24
30.	Resin identification codes	25
31.	Representations of some materials molecules	25
32.	Solubility product constants	26

33.	2-amino acids	27
34.	Lipids, carbohydrates and nucleotide components	29
35.	Vitamins and pigments	31
36.	Binding energy curve	33
37.	Representations of some medicinal molecules	34
38.	References	36

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	Topic	Equation
1.3	PV = nR	A.5	% Atom Economy = $\frac{\text{molar mass of desired product}}{\text{molar mass of all reactants}} \times 100\%$
2.2 and C.4	$c = v\lambda$	A.8	$n\lambda = 2dsin\theta$
5.1	$q=mc\Delta T$	B.7	$pH = pK_a + \log\left(\frac{[A^-]}{[HA]}\right)$
8.3	$pH = -\log_{10}[H_3O^+]$ or $pH = -\log_{10}[H^+]$	B.7	$\log_{10} \frac{I_0}{I} = \ \varepsilon lc$
12.1	E = hv	C.1	Energy density $=$ $\frac{\text{energy released from fuel}}{\text{volume of fuel consumed}}$
15.2	$\Delta G^{\circ} = \Delta H^{\circ} - T \Delta S^{\circ}$	C.1	Specific energy = $\frac{\text{energy released from fuel}}{\text{mass of fuel consumed}}$
16.2	$k = Ae^{\frac{-E_a}{RT}}$	C.3	$N = N_0 e^{-\lambda t}$
16.2	$\ln k = \frac{-E_a}{RT} + \ln A$	C.3 and D.8	$t_{\frac{1}{2}} = \frac{\ln 2}{\lambda}$
16.2	$\ln \frac{k_1}{k_2} = \frac{E_a}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$	C.6	$E = E^0 - \left(\frac{RT}{nF}\right) \ln Q$
17.1	$\Delta G^{\circ} = -RT \ln K$	C.7	$\frac{\text{Rate}_1}{\text{Rate}_2} = \sqrt{\frac{M_2}{M_1}}$
19.1	$\Delta G^{\circ} = -nFE^{\circ}$	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 × 10²³ mol⁻¹

Gas constant (R) = 8.31 J K⁻¹ mol⁻¹

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

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

STP conditions = 273 K and 100 kPa

SATP conditions = 298 K and 100 kPa

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

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

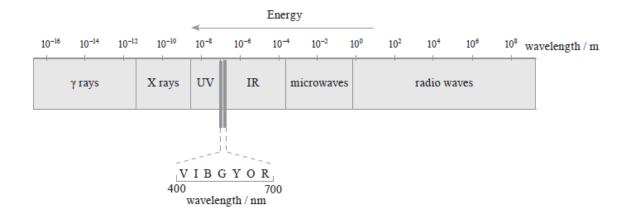
Planck's constant (h) = $6.63 \times 10^{-34} \text{ J s}$

Faraday's constant (F) = 96 500 C mol⁻¹

lonic product constant for water $(K_w) = 1.00 \times 10^{-14}$ at 298 K

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

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 × 10 ⁻¹⁹

5. Names of the elements

Element	Symbol	Atomic number	Element	Symbol	Atomic number
actinium	Ac	89	mendelevium	Md	101
aluminium	Al	13	mercury	Hg	80
americium	Am	95	molybdenum	Mo	42
antimony	Sb	51	neodymium	Nd	60
argon	Ar	18	neon	Ne	10
arsenic	As	33	neptunium	Np	93
astatine	At	85	nickel	Ni	28
barium	Ba	56	niobium	Nb	41
berkelium	Bk	97	nitrogen	N	7
beryllium	Be	4	nobelium	No	102
bismuth	Bi	83	osmium	Os	76
bohrium	Bh	107	oxygen	0	8
boron	В	5	palladium	Pd	46
bromine	Br	35	phosphorus	P	15
cadmium	Cd	48	platinum	Pt	78
caesium	Cs	55	plutonium	Pu	94
calcium	Ca	20	polonium	Po	84
californium	Cf	98	potassium	K	19
carbon	С	6	praseodymium	Pr	59
cerium	Ce	58	promethium	Pm	61
chlorine	Cl	17	protactinium	Pa	91
chromium	Cr	24	radium	Ra	88
cobalt	Co	27	radon	Rn	86
copernicium	Cn	112	rhenium	Re	75
copper	Cu	29	rhodium	Rh	45
curium	Cm	96	roentgenium	Rg	111
darmstadtium	Ds	110	rubidium	Rb	37
dubnium	Db	105	ruthenium	Ru	44
dysprosium	Dy	66	rutherfordium	Rf	104
einsteinium	Es	99	samarium	Sm	62
erbium	Er	68	scandium	Sc	21
europium	Eu	63	seaborgium	Sg	106
fermium	Fm	100	selenium	Se	34
fluorine	F	9	silicon	Si	14
francium	Fr	87	silver	Ag	47

Element	Symbol	Atomic number	Element	Symbol	Atomic number
gadolinium	Gd	64	sodium	Na	11
gallium	Ga	31	strontium	Sr	38
germanium	Ge	32	sulfur	S	16
gold	Au	79	tantalum	Ta	73
hafnium	Hf	72	technetium	Тс	43
hassium	Hs	108	tellurium	Te	52
helium	Не	2	terbium	Tb	65
holmium	Но	67	thallium	Tl	81
hydrogen	Н	1	thorium	Th	90
indium	In	49	thulium	Tm	69
iodine	I	53	tin	Sn	50
iridium	Ir	77	titanium	Ti	22
iron	Fe	26	tungsten	W	74
krypton	Kr	36	uranium	U	92
lanthanum	La	57	vanadium	V	23
lawrencium	Lr	103	xenon	Xe	54
lead	Pb	82	ytterbium	Yb	70
lithium	Li	3	yttrium	Y	39
lutetium	Lu	71	zinc	Zn	30
magnesium	Mg	12	zirconium	Zr	40
manganese	Mn	25			
meitnerium	Mt	109			

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																	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																	
				3.6.1.1	(0.5)												He
Н				Melting p	point (°C)												
-252.9		-		Flor	nent												-268.9
180.5	1287			Lici	Hent							2077	3500	-210.0	-218.8	-219.7	-248.6
Li	Be			Boiling p	point (°C)							В	C	N	О	F	Ne
1342	2468											4000	4827	-195.8	-183.0	-188.1	-246.0
97.8	650					<u>.</u>						660.3	1414	44.2	115.2	-101.5	-189.3
Na	Mg											Al	Si	P	S	Cl	Ar
114	wig											Ai	51	1		Ci	AI
882.9	1090							_				2519	3265	280.5	444.6	-34.0	-185.8
63.5	842	1541	1670	1910	1907	1246	1538	1495	1455	1084.6	419.5	29.8	938.2	817	220.8	-7.2	-157.4
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
759	1484	2836	3287	3407	2671	2061	2861	2927	2913	2560	907	2229	2833	616	685	58.8	-153.4
39.3	777	1522	1854	2477	2622	2157	2333	1963	1554.8	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	Te	I	Xe
688	1377	3345	4406	4741	4639	4262	4147	3695	2963	2162	767	2027	2586	1587	988	184.4	-108.1
28.5	727	920	2233	3017	3414	3453	3033	2446	1768.2	1064.2	-38.8	304	327.5	271.4	254	302	-71
C.	D.	T.o.	TIE	To	**/	D.	0	T	D4	A	TT.	TU	DI	D:	D.	At	D
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
671	1845	3464	4600	5455	5555	5900	5008	4428	3825	2836	356.6	1473	1749	1564	962		-61.7
21	696	1050															
Fr	Ra	Ac															

Chemistry data booklet

3200

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

1312 -73				First ioniz	ation	Elect	ron affinity	(kJ mol ⁻¹) A / kJ mol ⁻¹									2372
Н				energy (kJ mol ⁻¹)			Z EF	1 / KJ IIIOI									He
2.2																	
520 -60	900					Element						801 -27	1086 -122	1402	1314 -141	1681 -328	2081
Li	Be											В	C	N	(+753) O	\mathbf{F}	Ne
1.0	1.6				Ele	ctronegativ	vity					2.0	2.6	3.0	3.4	4.0	
496 -53	738		578 -42 787 -134 1012 -72 10												1000 -200	1251 -349	1520
Na	Mg											Al	Si	P	(+545) 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
0.8	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 -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	\mathbf{Zr}	Nb	Mo	Tc	Ru	Rh	Pd	$\mathbf{A}\mathbf{g}$	Cd	In	Sn	Sb	Te	I	Xe
0.8	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	503 -14	538 -45	659 -1	728 -31	759 -79	756 -14	814 -106	865 -151	864 -205	890 -223	1007	589 -36	716 -35	703 -91	812 -183	-270	1037
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
0.8	0.9	1.1	1.3	1.5	1.7	1.9	2.2	2.2	2.2	2.4	1.9	1.8	1.8	1.9	2.0	2.2	
393 -47	509 -10	499 -34		•	•			•			-			•			•
Fr	Ra	Ac															
0.7	0.9	1.1															

9. Atomic and ionic radii of the elements

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

10. Covalent bond lengths

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

	Br	С	CI	F	Н	I	N	0	Р	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
CI	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
Р	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 $(10^{-12} \text{ m} = \text{pm})$

C=C	134	C≡N	116	N≡N	110
C≡C	120	C=O	122	N=O	114
C === C	140	C=S	156	0=0	121
(in benzene)					
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	С	CI	F	Н	I	N	0	Р	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
CI	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
1	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
Р	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	507	C=S	536	0=0	498
(in benzene)					
C=N	615	N=N	470	S=S	429

12. Selected compounds—thermodynamic data

Substance	Formula	State	(kJ mol ⁻¹)	(kJ mol ⁻¹)	(J K ⁻¹ mol ⁻¹)
methane	CH ₄	g	-74.0	-50.0	+186
ethane	C ₂ H ₆	g	-84.0	-32.0	+230
propane	C ₃ H ₈	g	-105	-24.0	+270
butane	C ₄ H ₁₀	g	-126	-17.0	+310
pentane	C ₅ H ₁₂	1	-173		
hexane	C ₆ H ₁₄	1	-199		
ethene	C ₂ H ₄	g	+52.0	+68.0	+220
propene	C ₃ H ₆	g	+20.0	+62.0	+267
but-1-ene	C ₄ H ₈	g	+0.10	+71.0	+306
cis-but-2-ene	C ₄ H ₈	g	-7.0	+66.0	+301
trans-but-2-ene	C ₄ H ₈	g	-11.0	+63.0	+297
ethyne	C ₂ H ₂	g	+228	+211	+201
propyne	C ₃ H ₄	g	+185	+194	+248
buta-1,3-diene	C ₄ H ₆	g	+110	+151	+279
cyclohexane	C ₆ H ₁₂	1	-156		
benzene	C ₆ H ₆	1	+49.0	+125	+173
methylbenzene	C ₆ H ₅ CH ₃	1	+12.0		
ethylbenzene	C ₆ H ₅ CH ₂ CH ₃	1	-12.0		
phenylethene	C ₆ H ₅ CHCH ₂	1	+104		
chloromethane	CH₃CI	g	-82.0	-58.0	+235
dichloromethane	CH ₂ Cl ₂	1	-124		+178
trichloromethane	CHCl ₃	1	-134	-74.0	+202
bromomethane	CH₃Br	g	-36.0	-26.0	+246
iodomethane	CH₃I	1	-14.0		+163
chloroethane	C ₂ H ₅ Cl	g	-137	-53.0	
bromoethane	C₂H₅Br	I	-90.0	-26.0	+199
chlorobenzene	C ₆ H ₅ CI	I	+11.0		
methanol	CH₃OH	I	-239	-167	+127
ethanol	C ₂ H ₅ OH	I	-278	− 175	+161
phenol	C ₆ H ₅ OH	s	-165		+144
methanal	НСНО	g	-109	-102	+219
ethanal	CH₃CHO	g	-166	-133	+264
propanone	(CH ₃) ₂ CO	I	-248		+200
methanoic acid	нсоон	I	-425	-361	+129
ethanoic acid	CH₃COOH	1	-484	-390	+160
benzoic acid	C ₆ H ₅ COOH	s	-385		+168
methylamine	CH ₃ NH ₂	g	-23	+32.0	+243
water	H ₂ O	1	-285.8	-237.1	+70.0

Substance	Formula	State	(kJ mol ⁻¹)	(kJ mol ⁻¹)	(J K ⁻¹ mol ⁻¹)
steam	H ₂ O	g	-241.8	-228.6	+188.8
carbon monoxide	СО	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	HCI	g	-92.3	-95.3	+186.9
hydrogen fluoride	HF	g	-273.3	-275.4	+173.8
hydrogen iodide	н	g	+26.5	+1.7	+206.6

13. Enthalpies of combustion

The values of the molar enthalpy of combustion (ΔH_c°) in the following table refer to a temperature of 298 K and a pressure of 1.00 x 10⁵ Pa.

Substance	Formula	State	ΔH_c° (kJ mol ⁻¹)	Substance	Formula	State	ΔH_c° (kJ mol ⁻¹)
hydrogen	H_2	g	- 286	propan-1-ol	C ₃ H ₇ OH	1	-2021
sulfur	S	S	- 297	butan-1-ol	C ₄ H ₉ OH	1	- 2676
carbon (graphite)	С	S	- 394	cyclohexanol	$C_6H_{11}OH$	S	-3728
carbon monoxide	CO	g	- 283	phenol	C ₆ H ₅ OH	S	-3053
methane	CH ₄	g	- 891	ethoxyethane	$(C_2H_5)_2O$	1	-2724
ethane	C_2H_6	g	- 1561	methanal	НСНО	g	- 571
propane	C_3H_8	g	- 2219	ethanal	CH ₃ CHO	g	- 1167
butane	C_4H_{10}	g	- 2878	benzaldehyde	C ₆ H ₅ CHO	1	-3525
pentane	C_5H_{12}	1	- 3509	propanone	$(CH_3)_2CO$	1	- 1790
hexane	C_6H_{14}	1	- 4163	pentan-3-one	$(C_2H_5)_2CO$	1	-3100
octane	C_8H_{18}	1	- 5470	phenylethanone	CH ₃ COC ₆ H ₅	1	- 4149
cyclohexane	C_6H_{12}	1	- 3920	methanoic acid	НСООН	1	-255
ethene	C_2H_4	g	-1411	ethanoic acid	CH₃COOH	1	-874
buta-1,3-diene	C_4H_6	g	- 2541	benzoic acid	C ₆ H ₅ COOH	S	-3228
ethyne	C_2H_2	g	- 1301	ethanedioic acid	(COOH) ₂	S	-243
benzene	C_6H_6	1	- 3268	ethyl ethanoate	CH ₃ COOC ₂ H ₅	1	-2238
methylbenzene	$C_6H_5CH_3$	1	- 3910	ethanamide	CH ₃ CONH ₂	S	- 1186
naphthalene	$C_{10}H_{8}$	S	- 5156	methylamine	CH ₃ NH ₂	g	- 1086
chloroethane	C ₂ H ₅ Cl	g	-1413	phenylamine	$C_6H_5NH_2$	1	- 3393
iodoethane	C_2H_5I	1	- 1463	nitrobenzene	$C_6H_5NO_2$	1	-3088
trichloromethane	CHCl ₃	1	- 473	urea	$CO(NH_2)_2$	S	- 633
methanol	CH ₃ OH	1	- 726	glucose	$C_6H_{12}O_6$	S	-2803
ethanol	C ₂ H ₅ OH	1	- 1367	sucrose	$C_{12}H_{22}O_{11}$	S	- 5640

14. Common oxidation numbers of 3-D ions

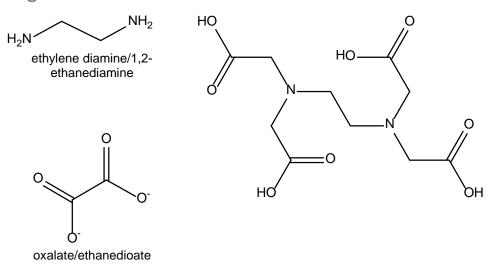
Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
								+1	
	+2	+2	+2	+2	+2	+2	+2	+2	+2
+3	+3	+3	+3	+3	+3	+3			
	+4	+4		+4					
		+5							
			+6	+6					
				+7					

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.

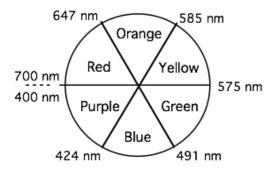
$$I^- < Br^- < S^{2-} < CI^- < F^- < OH^- < H_2O < SCN^- < NH_3 < CN^- < CO$$

16. Ligands



EDTA

17. Colour wheel



18. Lattice enthalpies at 298 K (experimental values)

The lattice enthalpy values $(\Delta H^{\circ}_{lattice})$ 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 this table are experimental values obtained by means of a suitable Born-Haber cycle.

Alkali metal halides				
	F	CI	Br	1
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	$\Delta H_{\rm lattice}^{\circ}$ (kJ mol ⁻¹)	Other subs	stances	$\Delta H_{\rm lattice}^{\circ}$ (kJ mol ⁻¹)
CaF ₂	2651	CuCl	2	2824
BeCl ₂	3033	AgF		974
MgCl ₂	2540	AgC	I	918
CaCl ₂	2271	AgBı	r	905
SrCl ₂	2170	AgI		892
BaCl ₂	2069			
MgO	3791			
CaO	3401			
SrO	3223			
ВаО	3054			

19. Enthalpies of aqueous solutions

Solute	$\Delta H_{\rm sol}^{\circ}$ (kJ mol ⁻¹)	Solute	$\Delta H_{ m sol}^{\circ}$ (kJ mol ⁻¹)
NH₄CI	+14.78	KCI	+17.22
NH ₄ NO ₃	+25.69	KBr	+19.87
LiF	+4.73	KI	+20.33
LiCl	-37.03	RbF	-26.11
LiBr	-48.83	RbCl	+17.28
Lil	-63.30	RbBr	+21.88
NaF	+0.91	RbI	+25.10
NaCl	+3.88	CsF	-36.86
NaBr	-0.60	CsCl	+17.78
Nal	-7.53	CsBr	+25.98
KF	-17.73	Csl	+33.35

20. Enthalpies of hydration

Cations	$\Delta H_{\mathrm{hyd}}^{\circ}(\mathrm{kJ\ mol}^{-1})$	Anions	$\Delta H_{\mathrm{hyd}}^{\circ}$ (kJ mol ⁻¹)
Li ⁺	-538	F ⁻	-504
Na ⁺	-424	Cl ⁻	-359
K ⁺	-340	Br ⁻	-328
Rb⁺	-315	Γ	-287
Cs⁺	-291	CIO ₃	-331
Be ²⁺	-2524	BrO ₃	-358
Mg ²⁺	-1963	IO ₃	-446
Ca ²⁺	-1616	CIO ₄	-205
Sr ²⁺	-1483	OH ⁻	-519
Ba ²⁺	-1346	CN ⁻	-341
Ra ²⁺	-1335	NO ₃	-316
Al ³⁺	-4741	HCO ₃	-383
Ga ³⁺	-4745	CO ₃ ²⁻	-1486
In ³⁺	-4171	HSO ₄	-362
Tl ³⁺	-4163	SO ₄ ²⁻	-1099
TI ⁺	-346	PO ₄ ³⁻	-2921
Sn ²⁺	-1587		
Pb ²⁺	-1523		

21. Strengths of organic acids and bases

The acid strengths in the following tables are given in terms of p K_a values, where p K_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	p <i>K</i> a
methanoic	HCOOH	3.75
ethanoic	CH₃COOH	4.76
propanoic	CH₃CH₂COOH	4.87
butanoic	CH ₃ (CH ₂) ₂ COOH	4.83
2-methylpropanoic	(CH ₃) ₂ CHCOOH	4.84
pentanoic	CH ₃ (CH ₂) ₃ COOH	4.83
2,2-dimethylpropanoic	(CH ₃) ₃ CCOOH	5.03
benzoic	C ₆ H ₅ COOH	4.20
phenylethanoic	$C_6H_5CH_2COOH$	4.31

Halogenated carboxylic acids

Name	Formula	p <i>K</i> a
chloroethanoic	CH₂CICOOH	2.87
dichloroethanoic	CHCl₂COOH	1.35
trichloroethanoic	CCl₃COOH	0.66
fluoroethanoic	CH₂FCOOH	2.59
bromoethanoic	CH₂BrCOOH	2.90
iodoethanoic	CH ₂ ICOOH	3.18

Phenols

Name	Formula	p <i>K</i> a
phenol	C ₆ H ₅ OH	9.99
2-nitrophenol	O ₂ NC ₆ H ₄ OH	7.23
3-nitrophenol	O ₂ NC ₆ H ₄ OH	8.36
4-nitrophenol	O ₂ NC ₆ H ₄ 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	p <i>K</i> a	
methanol	CH₃OH	15.5	
ethanol	C_2H_5OH	15.5	

Amines

Name	Formula	p <i>K</i> _b
ammonia	NH ₃	4.75
methylamine	CH ₃ NH ₂	3.34
ethylamine	CH ₃ CH ₂ NH ₂	3.35
dimethylamine	(CH ₃) ₂ NH	3.27
trimethylamine	(CH₃)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

			Co	lour change	
Indicator	p <i>K</i> _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. Ionization constant of water at varying temperatures

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

24. Standard electrode potentials (298 K)

Oxidized species	-	Reduced species	$E^{\circ}(V)$
$Li^+(aq) + e^-$		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
$H_2O(1) + e^-$		$\frac{1}{2}H_2(g) + OH^-(aq)$	-0.83
$Zn^{2+}(aq) + 2e^-$		Zn(s)	-0.76
$\mathrm{Fe}^{2+}(\mathrm{aq}) + 2\mathrm{e}^{-}$		Fe(s)	-0.45
$Ni^{2+}(aq) + 2e^-$		Ni(s)	-0.26
$\mathrm{Sn}^{2+}(\mathrm{aq}) + 2\mathrm{e}^{-}$		Sn(s)	-0.14
$Pb^{2+}(aq) + 2e^-$		Pb(s)	-0.13
$H^{+}(aq) + e^{-}$		$\frac{1}{2}H_{2}(g)$	0.00
$Cu^{2+}(aq) + e^-$		Cu ⁺ (aq)	+0.15
$SO_4^{2-}(aq) + 4H^+(aq) + 2e^-$		$H_2SO_3(\text{aq}) + H_2O(l)$	+0.17
$Cu^{2+}(aq) + 2e^-$		Cu(s)	+0.34
$^{1}/_{2}O_{2}(g) + H_{2}O(1) + 2e^{-}$		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
$^{1}/_{2}Br_{2}(1) + e^{-}$		Br ⁻ (aq)	+1.09
$^{1}/_{2}O_{2}(g) + 2H^{+}(aq) + 2e^{-}$		$H_2O(1)$	+1.23
${\rm Cr_2O_7}^{2-}({\rm aq}) + 14{\rm H^+}({\rm aq}) + 6{\rm e^-}$		$2Cr^{3+}(aq) + 7H_2O(1)$	+1.36
$^{1/2}Cl_{2}(g) + e^{-}$		Cl ⁻ (aq)	+1.36
$MnO_4^-(aq) + 8H^+(aq) + 5e^-$		$Mn^{2+}(\text{aq}) + 4H_2O(l)$	+1.51
$\frac{1}{2}F_{2}(g) + e^{-}$		F^{-} (aq)	+2.87

25. Activity series

Li Cs Rb K Ba Sr Ca Na Mg Be Al

Zn Cr Fe Cd Co Ni Sn Pb

Н

Sb

As Bi Cu Ag Pd Hg Pt Au

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-CI	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. ¹H 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.

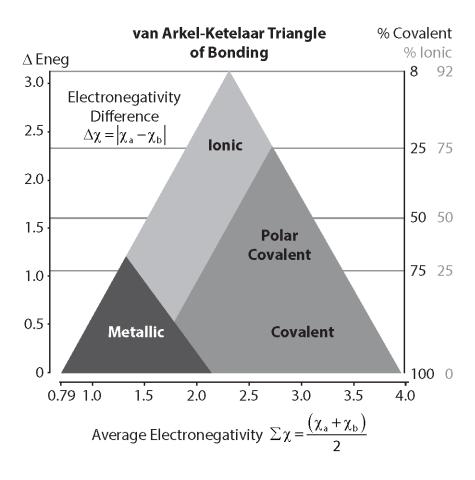
These values may vary in different solvents and conditions.

Type of proton	Chemical shift (ppm)
C H ₃	0.9–1.0
—СH ₂ -R	1.3–1.4
R ₂ CH	1.5
RO CH ₂	2.0–2.5
$R \stackrel{\text{O}}{\sim} CH_2$	2.2–2.7
$-$ C H $_3$	2.5–3.5
С≡С_Н	1.8–3.1
——CH ₂ -Hal	3.5–4.4
R_O_CH ₂ _	3.3–3.7
O R C O_CH ₂ _	3.7–4.8
R CO_H	9.0–13.0
R_O_ H	1.0–6.0
$HC=CH_2$	4.5–6.0
——ОН	4.0–12.0
—————Н	6.9–9.0
R H	9.4–10.0

28. Mass spectral fragments lost

Mass lost	Fragment lost	Mass lost	Fragment lost
15	CH₃·	29	CH₃CH₂·, CHO·
17	OH-	31	CH₃O·
18	H ₂ O	45	COOH-
28	CH ₂ =CH ₂ , C=O·		

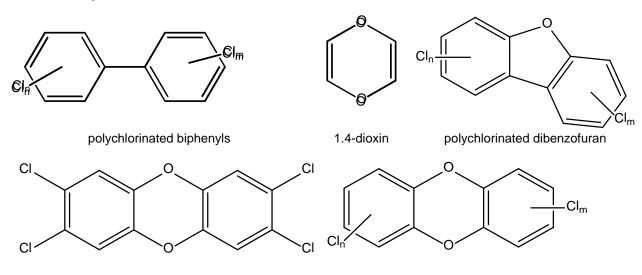
29. Triangular bonding diagram



30. Resin identification codes

Resin Identification Code (RIC)	Plastic types	Resin Identification Code (RIC)	Plastic types
PETE	polyethylene terephthalate	5 PP	polypropylene
ADPE HDPE	high-density polyethylene	<u>6</u>	polystyrene
23 PVC	polyvinyl chloride	OTHER	other
LDPE	low-density polyethylene		

31. Representations of some materials molecules



2,3,7,8-tetrachlorodibenzodioxin

polychlorinated dibenzo-p-dioxin

32. Solubility product constants (at 298 K)

Compound	K _{sp}	Compound	K sp
BaCO ₃	2.58 x 10 ⁻⁹	Hg ₂ CO ₃	3.6 x 10 ⁻¹⁷
Ba(OH) ₂ ·8H ₂ O	2.55 x 10 ⁻⁴	Hg₂SO₄	6.5 x 10 ⁻⁷
BaSO ₄	1.08 x 10 ⁻¹⁰	NiCO ₃	1.42 x 10 ⁻⁷
CdCO ₃	1.0 x 10 ⁻¹²	Ni(OH) ₂	5.48 x 10 ⁻¹⁶
Cd(OH) ₂	7.2 x 10 ⁻¹⁵	Ag ₂ CO ₃	8.46 x 10 ⁻¹²
PbCO ₃	7.40 x 10 ⁻¹⁴	Ag ₂ SO ₄	1.20 x 10 ⁻⁵
Pb(OH) ₂	1.43 x 10 ⁻²⁰	ZnCO ₃	1.46 x10 ⁻¹⁰
PbSO₄	2.53 x 10 ⁻⁸	Zn(OH) ₂	3 x 10 ⁻¹⁷

33. 2-amino acids

Common name	Symbol	Structural formula	pH of isoelectric point
alanine	Ala	H ₂ N—CH—COOH CH ₃	6.0
arginine	Arg	H_2N — CH — $COOH$ CH_2 — CH_2 — CH_2 — NH — C — NH_2 NH	10.8
asparagine	Asn	H ₂ N_CH_COOH CH ₂ _C_NH ₂	5.4
aspartic acid	Asp	H ₂ N—CH—COOH CH ₂ —COOH	2.8
cysteine	Cys	H ₂ N—CH—COOH CH ₂ —SH	5.1
glutamic acid	Glu	H ₂ N _ CH _ COOH CH ₂ _ CH ₂ _ COOH	3.2
glutamine	Gln	H ₂ N_CH_COOH CH ₂ -CH ₂ -C_NH ₂	5.7
glycine	Gly	H ₂ N—CH ₂ -COOH	6.0
histidine	His	H ₂ N—CH—COOH CH ₂ N H	7.6
isoleucine	lle	H ₂ N_CH_COOH H ₃ C_CH_CH ₂ -CH ₃	6.0
leucine	Leu	H ₂ N_CH_COOH CH ₂ H ₃ C_CH_CH ₃	6.0
lysine	Lys	H ₂ N_CH_COOH CH ₂ -CH ₂ -CH ₂ -NH ₂	9.7
methionine	Met	H ₂ N_CH_COOH CH ₂ -CH ₂ -S_CH ₃	5.7

Common name	Symbol	Structural formula	pH of isoelectric point
phenylalanine	Phe	H ₂ N=CH=COOH CH ₂	5.5
proline	Pro	COOH HN —	6.3
serine	Ser	H ₂ N—CH—COOH CH ₂ —OH	5.7
threonine	Thr	H ₂ N—CH—COOH H ₃ C—CH—OH	5.6
tryptophan	Тгр	H ₂ N_CH_COOH CH ₂	5.9
tyrosine	Tyr	H ₂ N=CH=COOH CH ₂	5.7
valine	Val	H ₂ N—CH—COOH H ₃ C—CH—CH ₃	6.0

34. Lipids, carbohydrates and nucleotide components

Lipids

Octanoic acid CH₃(CH₂)₆COOH

Lauric acid CH₃(CH₂)₁₀COOH

Palmitic acid CH₃(CH₂)₁₄COOH

Stearic acid CH₃(CH₂)₁₆COOH

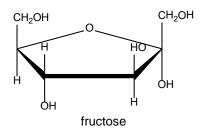
Oleic acid $CH_3(CH_2)_7CH = CH(CH_2)_7COOH$

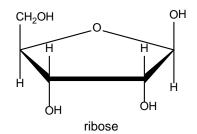
Linoleic acid $CH_3(CH_2)_4(CH = CHCH_2)_2(CH_2)_6COOH$

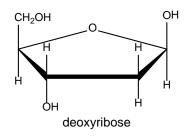
α-Linolenic acid $CH_3CH_2(CH) = CHCH_2(CH_2)_3(CH_2)_6COOH$

$$\begin{array}{c} H_3C \\ C \\ CH_3 \\ CH_3 \\ \end{array} \begin{array}{c} CH_2 \\ CH_2 \\ CH_3 \\ \end{array} \begin{array}{c} CH_2 \\ CH_3 \\ \end{array}$$

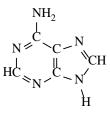
Carbohydrates



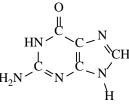


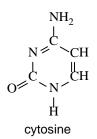


Nitrogenous bases



adenine





uracil

$$\begin{array}{c} O \\ H \\ N \\ C \\ C \\ CH \\ H \\ \text{thymine} \end{array}$$

35. Vitamins and pigments

Vitamins

$$\begin{array}{c} \text{CH}_3 & \text{CH}_3 & \text{CH}_3 \\ \text{CH} & \text{CH} & \text{CH} & \text{CH} \end{array} \\ \text{CH}_3 & \text{CH}_3 & \text{CH}_2 \\ \text{CH}_3 & \text{CH}_3 & \text{CH}_2 \\ \text{CH}_3 & \text{CH}_3 & \text{CH}_2 \end{array} \\ \text{retinol (vitamin A)} & \text{ascorbic acid (vitamin C)} \end{array}$$

$$\begin{array}{c} H_3C \setminus H \cdot CH_2 \cdot CH_2 \cdot CH_2 \cdot CH_3 \\ CH_3 \cdot CH_3 \cdot CH_2 \cdot CH_2 \cdot CH_3 \cdot CH_3 \cdot CH_3 \cdot CH_3 \cdot CH_2 \cdot CH_2 \cdot CH_2 \cdot CH_2 \cdot CH_2 \cdot CH_2 \cdot CH_3 \cdot CH_2 \cdot CH_2$$

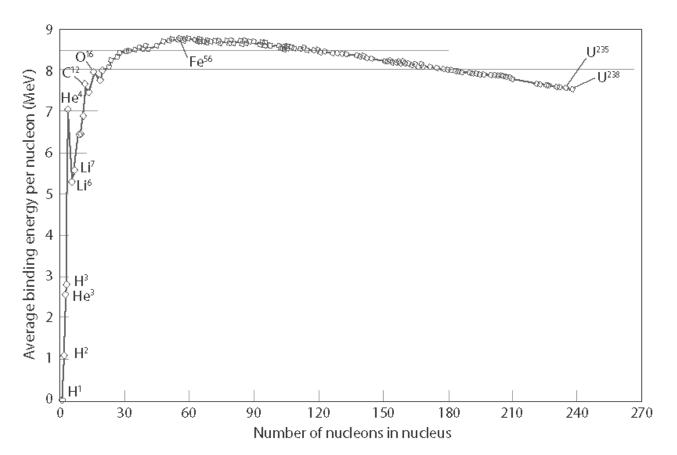
Pigments

Chemistry data booklet 32

α-carotene

$$H_3C$$
 CH_3
 CH_3
 CH_3
 CH_3
 CH_4
 CH_5
 CH_5

36. Binding energy curve



37. Representations of some medicinal molecules

$$H_3C-N$$
 C^2
 CH_2
 OH
 OH
 OH

diamorphine (heroin)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

penicillin (general structure)

paracetamol (acetaminophen)

$$H_3C-N$$
 C
 CH_2
 CH_3
 CH_3
 CH_3

omeprazole

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.