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Diploma Programme

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# Chemistry data booklet

First examinations 2009



**Diploma Programme  
Chemistry data booklet**

First published March 2007  
Revised edition published September 2008

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## Notes

This booklet cannot be used for paper 1 of the examination (SLP1 and HLP1), but the periodic table given on page 3 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, SLP3, HLP2 and HLP3).



## 1. Some relevant equations

$$\log_{10} \frac{I_0}{I} = \epsilon lc$$

$$k = A e^{-\frac{E_a}{RT}}$$

$$\ln k = -\frac{E_a}{RT} + \ln A$$

$$c=f\lambda$$

$$PV = nRT$$

$$\Delta G^\ominus = \Delta H^\ominus - T\Delta S^\ominus$$

$$q=mc\Delta T$$

$$E=hf$$

## 2. Physical constants and unit conversions

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

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

Molar volume of an ideal gas at 273 K and  $1.01 \times 10^5$  Pa =  $2.24 \times 10^{-2}$  m $^3$  mol $^{-1}$  (= 22.4 dm $^3$  mol $^{-1}$ )

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

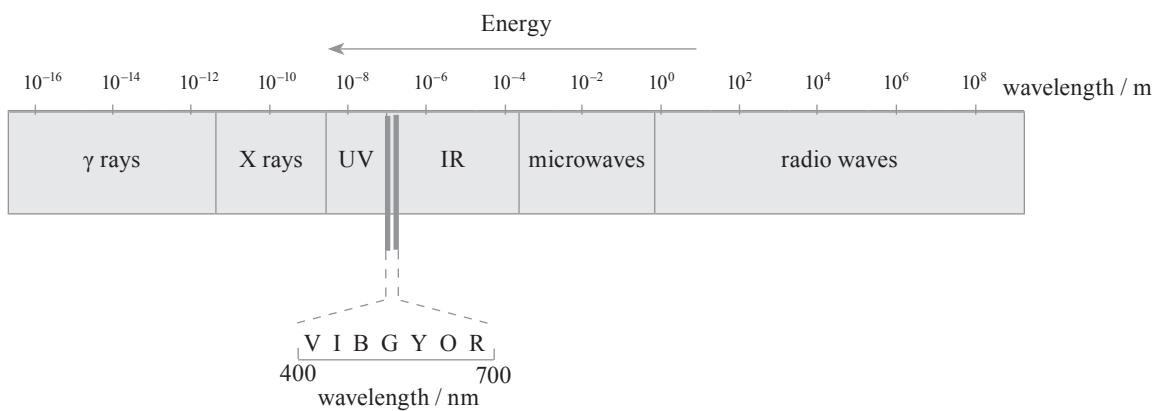
Specific heat capacity of water =  $4.18$  kJ kg $^{-1}$  K $^{-1}$  (=  $4.18$  J g $^{-1}$  K $^{-1}$ )

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

1 atm =  $1.01 \times 10^5$  Pa

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

## 3. The electromagnetic spectrum



## 4. 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	O	8
boron	B	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	C	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
copper	Cu	29	rhenium	Re	75
curium	Cm	96	rhodium	Rh	45
dubnium	Db	105	rubidium	Rb	37
dysprosium	Dy	66	ruthenium	Ru	44
einsteinium	Es	99	rutherfordium	Rf	104
erbium	Er	68	samarium	Sm	62
europium	Eu	63	scandium	Sc	21
fermium	Fm	100	seaborgium	Sg	106
fluorine	F	9	selenium	Se	34
francium	Fr	87	silicon	Si	14
gadolinium	Gd	64	silver	Ag	47
gallium	Ga	31	sodium	Na	11
germanium	Ge	32	strontium	Sr	38
gold	Au	79	sulfur	S	16
hafnium	Hf	72	tantalum	Ta	73
hassium	Hs	108	technetium	Tc	43
helium	He	2	tellurium	Te	52
holmium	Ho	67	terbium	Tb	65
hydrogen	H	1	thallium	Tl	81
indium	In	49	thorium	Th	90
iodine	I	53	thulium	Tm	69
iridium	Ir	77	tin	Sn	50
iron	Fe	26	titanium	Ti	22
krypton	Kr	36	tungsten	W	74
lanthanum	La	57	uranium	U	92
lawrencium	Lr	103	vanadium	V	23
lead	Pb	82	xenon	Xe	54
lithium	Li	3	ytterbium	Yb	70
lutetium	Lu	71	yttrium	Y	39
magnesium	Mg	12	zinc	Zn	30
manganese	Mn	25	zirconium	Zr	40
meitnerium	Mt	109			

## 5. The periodic table

	1	2	3	4	5	6	7	0
1	1 H 1.01	3 Li 6.94	4 Be 9.01					2 He 4.00
2				Element	Atomic number			
3	11 Na 22.99	12 Mg 24.31		Relative atomic mass				
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.90	23 Cr 50.94	24 Mn 52.00	25 Fe 54.94	26 Co 55.85
5	37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Nb 91.22	41 Zr 92.91	42 Mo 95.94	43 Tc 98.91	44 Ru 101.07
6	55 Cs 132.91	56 Ba 137.33	57 † La 138.91	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.21	76 Os 190.23
7	87 Fr 223.02	88 Ra 226.03	89 ‡ Ac 227.03	104 Rf 260	105 Db 262.11	106 Sg 266.12	107 Bh 264.12	109 Mt 269.13
				†	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm 144.91
					62 Sm 150.35	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 173.04	71 Lu 174.97		
				‡	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np 239.05
					94 Pu 239.05	95 Am 243.06	96 Cm 247.07	97 Bk 247.07
					98 Cf 252.08	99 Es 254.09	100 Fm 253.09	101 Md 257.10
					102 No 255.09	103 Lr 257		

## 6. Melting points and boiling points of the elements

	Melting point / K	Boiling point / K
Element		
<b>H</b>	14	20
<b>Li</b>	454	1551
<b>Be</b>	1615	3243
<b>Na</b>	371	922
<b>Mg</b>	1156	1380
<b>K</b>	336	1112
<b>Ca</b>	1033	1757
<b>Sc</b>	3104	1814
<b>Ti</b>	3560	1933
<b>V</b>	3653	2163
<b>Cr</b>	2943	2130
<b>Mn</b>	2235	1517
<b>Fe</b>	3023	1808
<b>Co</b>	3143	1768
<b>Ni</b>	3003	1728
<b>Cu</b>	2840	1356
<b>Zn</b>	1180	693
<b>Ga</b>	2676	303
<b>Ge</b>	3103	1210
<b>As</b>	886	1090
<b>Se</b>	958	490
<b>Br</b>	332	266
<b>Kr</b>	121	116
<b>Rb</b>	312	1042
<b>Sr</b>	959	1795
<b>Y</b>	3611	2125
<b>Zr</b>	4650	2740
<b>Nb</b>	5015	2883
<b>Mo</b>	5833	2445
<b>Tc</b>	5150	2583
<b>Ru</b>	4173	2239
<b>Rh</b>	4000	1827
<b>Pd</b>	3243	1235
<b>Ag</b>	2485	594
<b>Cd</b>	1038	429
<b>In</b>	2353	505
<b>Sn</b>	2543	904
<b>Sb</b>	2023	723
<b>Te</b>	1263	387
<b>I</b>	457	161
<b>Xe</b>	166	161
<b>Cs</b>	302	998
<b>Ba</b>	942	1194
<b>La</b>	3730	2500
<b>Hf</b>	4875	3269
<b>Ta</b>	5700	3683
<b>Re</b>	5900	3453
<b>W</b>	5933	2973
<b>Os</b>	5570	2683
<b>Tl</b>	630	1337
<b>Hg</b>	4403	2045
<b>Au</b>	3353	1337
<b>Pt</b>	4100	577
<b>Ir</b>	1730	601
<b>Pb</b>	2013	544
<b>Bi</b>	1833	527
<b>Po</b>	1235	575
<b>At</b>	610	202
<b>Rn</b>	211	202
<b>Fr</b>	300	973
<b>Ra</b>	950	1323
<b>Ac</b>	1413	3473

Element
---------

	1 <b>He</b> 4
<b>B</b>	2573
<b>C</b>	3925
<b>N</b>	63
<b>O</b>	90
<b>F</b>	55
<b>S</b>	95
<b>Cl</b>	53
<b>Ar</b>	85
<b>Ne</b>	25
<b>He</b>	27

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

		First ionization energy / kJ mol <sup>-1</sup>		Electron affinity / kJ mol <sup>-1</sup> 2 <sup>nd</sup> EA / kJ mol <sup>-1</sup>	
		Element Electronegativity			
1312	-73				
<b>H</b>	2.2				
520	-60	900	<b>Be</b>		
<b>Li</b>	1.0	1.6			
496	-53	738	<b>Na</b>		
<b>Mg</b>	0.9	1.3			
419	-48	590	-2	631	-18
<b>K</b>	0.8	<b>Ca</b>	Sc	Ti	V
403	47	550	-5	616	-30
<b>Rb</b>	0.8	<b>Sr</b>	Y	Nb	Zr
376	-46	503	-14	538	-45
<b>Cs</b>	0.8	<b>Ba</b>	La	Hf	Ta
393	-44	509	-10	499	-34
<b>Fr</b>	0.7	<b>Ra</b>	<b>Ac</b>		

		First ionization energy / kJ mol <sup>-1</sup>		Electron affinity / kJ mol <sup>-1</sup> 2 <sup>nd</sup> EA / kJ mol <sup>-1</sup>	
		Element			
1312	-73				
<b>He</b>	2372				
801	-27	1086	-122	1402	1314 +798
<b>B</b>	2.0	<b>C</b>	<b>N</b>	<b>O</b>	<b>F</b>
578	-42	789	-134	1012 +640	1251 -349
<b>Al</b>	1.6	<b>Si</b>	<b>P</b>	<b>S</b>	<b>Cl</b>
579	-41	762	-119	947 -200	941 -195
<b>Ge</b>	1.8	<b>As</b>	<b>Se</b>	<b>Br</b>	<b>Kr</b>
558	-29	709	-107	834 -101	869 -190
<b>In</b>	1.7	<b>Sn</b>	<b>Te</b>	<b>I</b>	<b>Xe</b>
589	-19	716	-35	703 -223	91 -183
<b>Pt</b>	2.2	<b>Au</b>	<b>Hg</b>	<b>Po</b>	<b>At</b>
393	-44	509	-10	499 -34	2.0 2.2
<b>Fr</b>	0.7	<b>Ra</b>	<b>Ac</b>		

## 8. Atomic and ionic radii of the elements

Element	Atomic radius / $10^{-12}$ m	Ionic radius / $10^{-12}$ m
<b>H</b>	30	112
<b>Li</b>	152 154 (1-)	<b>Be</b> 112
<b>B</b>	68 (1+)	30 (2+)

	<b>He</b>
<b>B</b>	88 C 16 (3+)
<b>Al</b>	143 42 (4+) 271 (4-)
<b>Ga</b>	141 53 (4+) 272 (4-)
<b>In</b>	166 112 (2+) 71 (4+)
<b>Tl</b>	171 150 (1+) 93 (3+)
<b>C</b>	77 260 (4-)
<b>Si</b>	117 212 (3-)
<b>Ge</b>	122 222 (3-)
<b>Sn</b>	162 112 (2+) 71 (4+)
<b>Pb</b>	175 120 (2+) 84 (4+)
<b>N</b>	70 171 (3-)
<b>P</b>	110 190 (2-)
<b>As</b>	121 202 (2-)
<b>Sb</b>	141 245 (3-)
<b>Bi</b>	170 120 (3+) 76 (5+)
<b>O</b>	66 146 (2-)
<b>S</b>	104 190 (2-)
<b>Se</b>	117 222 (2-)
<b>Te</b>	137 219 (1-)
<b>F</b>	99 133 (1-)
<b>Cl</b>	114 181 (1-)
<b>Br</b>	114 196 (1-)
<b>I</b>	133 219 (1-)
<b>Xe</b>	140 140
<b>Ne</b>	64
<b>Ar</b>	99
<b>Kr</b>	114
<b>Rn</b>	62 (7+)

Fr	180 (1+)	270	188
		220	112 (3+)

## 9. Covalent bond lengths

Bond	Bond length / nm	Bond	Bond length / nm
H–H	0.074	C–H	0.108
C–C	0.154	Si–H	0.148
C=C	0.134	N–H	0.101
C≡C	0.120	P–H	0.144
C=C (in benzene)	0.140	O–H	0.096
Si–Si	0.235	S–H	0.134
N–N	0.145	F–H	0.092
N=N	0.120	Cl–H	0.127
N≡N	0.110	Br–H	0.141
P–P	0.221	I–H	0.161
O–O	0.148	C–O	0.143
O=O	0.121	C=O	0.120
S–S	0.205	C–N	0.147
S=S	0.189	C=N	0.130
F–F	0.142	C≡N	0.116
Cl–Cl	0.199	C–F	0.138
Br–Br	0.228	C–Cl	0.177
I–I	0.267	C–Br	0.194
		C–I	0.214
		Si–O	0.161

## 10. Bond enthalpies and average bond enthalpies at 298 K

Bond	$\Delta H / \text{kJ mol}^{-1}$	Bond	$\Delta H / \text{kJ mol}^{-1}$
H–H	436	C–H	413
C–C	347	Si–H	318
C=C	612	N–H	391
C≡C	838	P–H	321
C=C (benzene)	505	O–H	464
Si–Si	226	S–H	364
N–N	158	F–H	568
N=N	410	Cl–H	432
N≡N	945	Br–H	366
P–P	198	I–H	298
O–O	144		
O=O	498	C–O	358
S–S	266	C=O	746
F–F	158	C–N	286
Cl–Cl	243	C=N	615
Br–Br	193	C≡N	887
I–I	151	C–F	467
		C–Cl	346
		C–Br	290
		C–I	228
		Si–O	466

# 11. Organic compounds—thermodynamic data

Substance	Formula	State	$\Delta H_f^\ominus / \text{kJ mol}^{-1}$	$\Delta G_f^\ominus / \text{kJ mol}^{-1}$	$S^\ominus / \text{J K}^{-1} \text{ mol}^{-1}$
methane	CH <sub>4</sub>	g	-75	-51	186
ethane	C <sub>2</sub> H <sub>6</sub>	g	-85	-33	230
propane	C <sub>3</sub> H <sub>8</sub>	g	-105	-23	270
butane	C <sub>4</sub> H <sub>10</sub>	g	-127	-16	310
pentane	C <sub>5</sub> H <sub>12</sub>	l	-173	-9	261
hexane	C <sub>6</sub> H <sub>14</sub>	l	-199	-4	296
ethene	C <sub>2</sub> H <sub>4</sub>	g	52	68	220
propene	C <sub>3</sub> H <sub>6</sub>	g	20	75	267
but-1-ene	C <sub>4</sub> H <sub>8</sub>	g	0*	72	306
<i>cis</i> -but-2-ene	C <sub>4</sub> H <sub>8</sub>	g	-8	66	301
<i>trans</i> -but-2-ene	C <sub>4</sub> H <sub>8</sub>	g	-12	63	296
ethyne	C <sub>2</sub> H <sub>2</sub>	g	228	209	201
propyne	C <sub>3</sub> H <sub>4</sub>	g	187	194	248
buta-1,3-diene	C <sub>4</sub> H <sub>6</sub>	g	110	152	279
cyclohexane	C <sub>6</sub> H <sub>12</sub>	l	-156	27	204
benzene	C <sub>6</sub> H <sub>6</sub>	l	49	125	173
methylbenzene	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	l	12	111	320
ethylbenzene	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> CH <sub>3</sub>	l	-13	120	255
phenylethene	C <sub>6</sub> H <sub>5</sub> CHCH <sub>2</sub>	l	104	203	345
chloromethane	CH <sub>3</sub> Cl	g	-82	-57	235
dichloromethane	CH <sub>2</sub> Cl <sub>2</sub>	l	-124	-63	178
trichloromethane	CHCl <sub>3</sub>	l	-135	-71	202
bromomethane	CH <sub>3</sub> Br	g	-37	-26	246
iodomethane	CH <sub>3</sub> I	l	-16	13	163
chloroethane	C <sub>2</sub> H <sub>5</sub> Cl	g	-137	-53	
bromoethane	C <sub>2</sub> H <sub>5</sub> Br	l	-91		
chlorobenzene	C <sub>6</sub> H <sub>5</sub> Cl	l	11	94	
methanol	CH <sub>3</sub> OH	l	-239	-166	240
ethanol	C <sub>2</sub> H <sub>5</sub> OH	l	-277	-175	161
phenol	C <sub>6</sub> H <sub>5</sub> OH	s	-165	-48	
methanal	HCHO	g	-109	-113	219
ethanal	CH <sub>3</sub> CHO	g	-191	-128	160
propanone	(CH <sub>3</sub> ) <sub>2</sub> CO	l	-248	-155	
methanoic acid	HCOOH	l	-425	-361	129
ethanoic acid	CH <sub>3</sub> COOH	l	-485	-390	160
benzoic acid	C <sub>6</sub> H <sub>5</sub> COOH	s	-385	-245	
methylamine	CH <sub>3</sub> NH <sub>2</sub>	g	-23	32	243

\* (-0.4)

## 12. 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  $1.01 \times 10^5$  Pa (1 atm).

Substance	Formula	State	$\Delta H_c^\ominus / \text{kJ mol}^{-1}$
hydrogen	H <sub>2</sub>	g	-286
sulfur	S	s	-297
carbon (graphite)	C	s	-394
carbon monoxide	CO	g	-283
methane	CH <sub>4</sub>	g	-890
ethane	C <sub>2</sub> H <sub>6</sub>	g	-1560
propane	C <sub>3</sub> H <sub>8</sub>	g	-2219
butane	C <sub>4</sub> H <sub>10</sub>	g	-2877
pentane	C <sub>5</sub> H <sub>12</sub>	l	-3509
hexane	C <sub>6</sub> H <sub>14</sub>	l	-4163
octane	C <sub>8</sub> H <sub>18</sub>	l	-5470
cyclohexane	C <sub>6</sub> H <sub>12</sub>	l	-3920
ethene	C <sub>2</sub> H <sub>4</sub>	g	-1411
buta-1,3-diene	C <sub>4</sub> H <sub>6</sub>	g	-2541
ethyne	C <sub>2</sub> H <sub>2</sub>	g	-1301
benzene	C <sub>6</sub> H <sub>6</sub>	l	-3267
methylbenzene	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	l	-3910
naphthalene	C <sub>10</sub> H <sub>8</sub>	s	-5156
chloroethane	C <sub>2</sub> H <sub>5</sub> Cl	g	-1413
bromoethane	C <sub>2</sub> H <sub>5</sub> Br	l	-1425
iodoethane	C <sub>2</sub> H <sub>5</sub> I	l	-1467
(chloromethyl)benzene	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> Cl	l	-3709
trichloromethane	CHCl <sub>3</sub>	l	-474
methanol	CH <sub>3</sub> OH	l	-726
ethanol	C <sub>2</sub> H <sub>5</sub> OH	l	-1367

Substance	Formula	State	$\Delta H_c^\ominus / \text{kJ mol}^{-1}$
propan-1-ol	C <sub>3</sub> H <sub>7</sub> OH	l	-2021
butan-1-ol	C <sub>4</sub> H <sub>9</sub> OH	l	-2676
cyclohexanol	C <sub>6</sub> H <sub>11</sub> OH	s	-3727
phenol	C <sub>6</sub> H <sub>5</sub> OH	s	-3053
ethoxyethane	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	l	-2724
methanal	HCHO	g	-571
ethanal	CH <sub>3</sub> CHO	g	-1167
benzaldehyde	C <sub>6</sub> H <sub>5</sub> CHO	l	-3525
propanone	(CH <sub>3</sub> ) <sub>2</sub> CO	l	-1817
pentan-3-one	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	l	-3100
phenylethanone	CH <sub>3</sub> COC <sub>6</sub> H <sub>5</sub>	l	-4149
methanoic acid	HCOOH	l	-254
ethanoic acid	CH <sub>3</sub> COOH	l	-874
benzoic acid	C <sub>6</sub> H <sub>5</sub> COOH	s	-3227
ethanedioic acid	(COOH) <sub>2</sub>	s	-243
ethyl ethanoate	CH <sub>3</sub> COOC <sub>2</sub> H <sub>5</sub>	l	-2238
ethanamide	CH <sub>3</sub> CONH <sub>2</sub>	s	-1185
methylamine	CH <sub>3</sub> NH <sub>2</sub>	g	-1085
ethylamine	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	g	-1740
phenylamine	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	l	-3393
nitrobenzene	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	l	-3088
urea	CO(NH <sub>2</sub> ) <sub>2</sub>	s	-632
glucose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	s	-2803
sucrose	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	s	-5640

## 13. Lattice enthalpies at 298 K (experimental and theoretical values)

The lattice enthalpy values ( $\Delta H_{\text{lattice}}^{\ominus}$ ) given relate to the endothermic process for a solid crystal breaking into gaseous ions.

For example, for an alkali metal halide:



### Experimental values

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

Alkali metal halides	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$			
	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	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$	Other substances	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$
CaF <sub>2</sub>	2651	CuCl <sub>2</sub>	2824
BeCl <sub>2</sub>	3033	AgF	974
MgCl <sub>2</sub>	2540	AgCl	918
CaCl <sub>2</sub>	2271	AgBr	905
SrCl <sub>2</sub>	2170	AgI	892
BaCl <sub>2</sub>	2069		
MgO	3791		
CaO	3401		
SrO	3223		
BaO	3054		

## Theoretical values

These two tables contain lattice enthalpies calculated from electrostatic principles on the basis of a purely ionic model for the crystal.

Alkali metal halides	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$			
	F	Cl	Br	I
Li	1030	834	788	730
Na	910	769	732	682
K	808	701	671	632
Rb	774	680	651	617
Cs	744	657	632	600
Other substances	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$	Other substances	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$	
CaF <sub>2</sub>	2640	AgF	953	
MgO	3795	AgCl	910	
CaO	3414	AgBr	897	
SrO	3217	AgI	881	
BaO	3029			

## 14. Standard electrode potentials

Oxidized species		Reduced species	$E^\ominus / \text{V}$
$\text{Li}^+(\text{aq}) + \text{e}^-$	$\rightleftharpoons$	$\text{Li(s)}$	-3.04
$\text{K}^+(\text{aq}) + \text{e}^-$	$\rightleftharpoons$	$\text{K(s)}$	-2.93
$\text{Ca}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Ca(s)}$	-2.87
$\text{Na}^+(\text{aq}) + \text{e}^-$	$\rightleftharpoons$	$\text{Na(s)}$	-2.71
$\text{Mg}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Mg(s)}$	-2.37
$\text{Al}^{3+}(\text{aq}) + 3\text{e}^-$	$\rightleftharpoons$	$\text{Al(s)}$	-1.66
$\text{Mn}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Mn(s)}$	-1.19
$\text{H}_2\text{O(l)} + \text{e}^-$	$\rightleftharpoons$	$\frac{1}{2}\text{H}_2(\text{g}) + \text{OH}^-(\text{aq})$	-0.83
$\text{Zn}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Zn(s)}$	-0.76
$\text{Fe}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Fe(s)}$	-0.45
$\text{Ni}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Ni(s)}$	-0.26
$\text{Sn}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Sn(s)}$	-0.14
$\text{Pb}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Pb(s)}$	-0.13
$\text{H}^+(\text{aq}) + \text{e}^-$	$\rightleftharpoons$	$\frac{1}{2}\text{H}_2(\text{g})$	0.00
$\text{Cu}^{2+}(\text{aq}) + \text{e}^-$	$\rightleftharpoons$	$\text{Cu}^+(\text{aq})$	+0.15
$\text{SO}_4^{2-}(\text{aq}) + 4\text{H}^+(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{H}_2\text{SO}_3(\text{aq}) + \text{H}_2\text{O(l)}$	+0.17
$\text{Cu}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Cu(s)}$	+0.34
$\frac{1}{2}\text{O}_2(\text{g}) + \text{H}_2\text{O(l)} + 2\text{e}^-$	$\rightleftharpoons$	$2\text{OH}^-(\text{aq})$	+0.40
$\text{Cu}^+(\text{aq}) + \text{e}^-$	$\rightleftharpoons$	$\text{Cu(s)}$	+0.52
$\frac{1}{2}\text{I}_2(\text{s}) + \text{e}^-$	$\rightleftharpoons$	$\text{I}^-(\text{aq})$	+0.54
$\text{Fe}^{3+}(\text{aq}) + \text{e}^-$	$\rightleftharpoons$	$\text{Fe}^{2+}(\text{aq})$	+0.77
$\text{Ag}^+(\text{aq}) + \text{e}^-$	$\rightleftharpoons$	$\text{Ag(s)}$	+0.80
$\frac{1}{2}\text{Br}_2(\text{l}) + \text{e}^-$	$\rightleftharpoons$	$\text{Br}^-(\text{aq})$	+1.07
$\frac{1}{2}\text{O}_2(\text{g}) + 2\text{H}^+(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{H}_2\text{O(l)}$	+1.23
$\text{Cr}_2\text{O}_7^{2-}(\text{aq}) + 14\text{H}^+(\text{aq}) + 6\text{e}^-$	$\rightleftharpoons$	$2\text{Cr}^{3+}(\text{aq}) + 7\text{H}_2\text{O(l)}$	+1.33
$\frac{1}{2}\text{Cl}_2(\text{g}) + \text{e}^-$	$\rightleftharpoons$	$\text{Cl}^-(\text{aq})$	+1.36
$\text{MnO}_4^-(\text{aq}) + 8\text{H}^+(\text{aq}) + 5\text{e}^-$	$\rightleftharpoons$	$\text{Mn}^{2+}(\text{aq}) + 4\text{H}_2\text{O(l)}$	+1.51
$\frac{1}{2}\text{F}_2(\text{g}) + \text{e}^-$	$\rightleftharpoons$	$\text{F}^-(\text{aq})$	+2.87

## 15. 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 <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	$pK_a$
chloroethanoic	CH <sub>2</sub> ClCOOH	2.87
dichloroethanoic	CHCl <sub>2</sub> COOH	1.35
trichloroethanoic	CCl <sub>3</sub> COOH	0.66
fluoroethanoic	CH <sub>2</sub> FCOOH	2.59
bromoethanoic	CH <sub>2</sub> BrCOOH	2.90
iodoethanoic	CH <sub>2</sub> I COOH	3.18

### Phenols

Name	Formula	$pK_a$
phenol	C <sub>6</sub> H <sub>5</sub> OH	9.99
2-nitrophenol	O <sub>2</sub> N C <sub>6</sub> H <sub>4</sub> OH	7.23
3-nitrophenol	O <sub>2</sub> N C <sub>6</sub> H <sub>3</sub> OH	8.36
4-nitrophenol	O <sub>2</sub> N C <sub>6</sub> H <sub>5</sub> OH	7.15
2,4-dinitrophenol	(O <sub>2</sub> N) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> OH	4.07
2,4,6-trinitrophenol	(O <sub>2</sub> N) <sub>3</sub> C <sub>6</sub> H <sub>2</sub> OH	0.42

## Alcohols

Name	Formula	$pK_a$
methanol	CH <sub>3</sub> OH	15.5
ethanol	C <sub>2</sub> H <sub>5</sub> OH	15.5

## Amines

Name	Formula	$pK_b$
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 <sub>3</sub> ) <sub>3</sub> N	4.20
diethylamine	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH	3.16
triethylamine	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	3.25
phenylamine	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	9.13

## 16. Acid–base indicators

Indicator	$pK_a$	pH range	Colour change	
			Acid	Alkali
methyl orange	3.46	3.2–4.4	red	yellow
bromophenol blue	4.10	3.0–4.6	yellow	blue
bromocresol green	4.90	3.8–5.4	yellow	blue
methyl red	5.00	4.8–6.0	red	yellow
bromothymol blue	7.30	6.0–7.6	yellow	blue
phenol red	8.00	6.6–8.0	yellow	red
phenolphthalein	9.50	8.2–10.0	colourless	pink

## 17. Infrared data

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

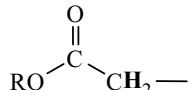
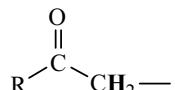
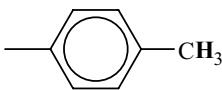
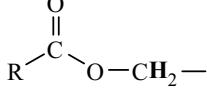
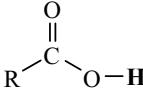
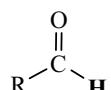
Bond	Organic molecules	Wavenumber / cm <sup>-1</sup>
C—I	iodoalkanes	490–620
C—Br	bromoalkanes	500–600
C—Cl	chloroalkanes	600–800
C—F	fluoroalkanes	1000–1400
C—O	alcohols, esters, ethers	1050–1410
C=C	alkenes	1610–1680
C=O	aldehydes, ketones, carboxylic acids and esters	1700–1750
C≡C	alkynes	2100–2260
O—H	hydrogen bonding in carboxylic acids	2500–3300
C—H	alkanes, alkenes, arenes	2850–3100
O—H	hydrogen bonding in alcohols and phenols	3200–3600
N—H	primary amines	3300–3500

## 18. $^1\text{H}$ NMR data

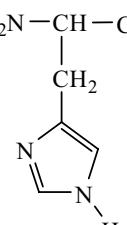
Typical proton chemical shift values ( $\delta$ ) relative to tetramethylsilane (TMS) = 0.

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

These values may vary in different solvents and conditions.

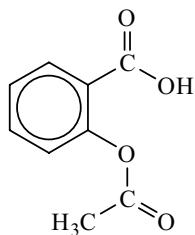
Type of proton	Chemical shift / ppm
$-\text{CH}_3$	0.9–1.0
$-\text{CH}_2-\text{R}$	1.3–1.4
$-\text{CHR}_2$	1.4–1.6
	2.0–2.5
	2.2–2.7
	2.5–3.5
$-\text{C}\equiv\text{C}-\text{H}$	1.8–3.1
$-\text{CH}_2-\text{Hal}$	3.5–4.4
$\text{R}-\text{O}-\text{CH}_2-$	3.3–3.7
	3.8–4.1
	9.0–13.0
$\text{R}-\text{O}-\text{H}$	4.0–12.0
$-\text{HC}=\text{CH}_2$	4.5–6.0
	4.0–12.0
	6.9–9.0
	9.4–10.0

## 19. 2-Amino acids

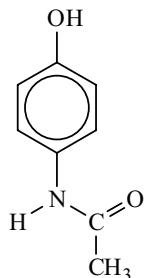
Common name	Symbol	Structural formula	pH of isoelectric point
alanine	Ala	$\text{H}_2\text{N}-\underset{\text{CH}_3}{\text{CH}}-\text{COOH}$	6.0
arginine	Arg	$\text{H}_2\text{N}-\underset{\text{CH}_2-\text{CH}_2-\text{CH}_2}{\text{CH}}-\text{NH}-\underset{\text{NH}}{\underset{\parallel}{\text{C}}}-\text{NH}_2$	10.8
asparagine	Asn	$\text{H}_2\text{N}-\underset{\text{CH}_2-\underset{\text{O}}{\underset{\parallel}{\text{C}}}-\text{NH}_2}{\underset{\text{CH}_2}{\text{CH}}}-\text{COOH}$	5.4
aspartic acid	Asp	$\text{H}_2\text{N}-\underset{\text{CH}_2-\text{COOH}}{\underset{\text{CH}_2}{\text{CH}}}-\text{COOH}$	2.8
cysteine	Cys	$\text{H}_2\text{N}-\underset{\text{CH}_2-\text{SH}}{\underset{\text{CH}_2}{\text{CH}}}-\text{COOH}$	5.1
glutamic acid	Glu	$\text{H}_2\text{N}-\underset{\text{CH}_2-\text{CH}_2-\text{COOH}}{\underset{\text{CH}_2}{\text{CH}}}-\text{COOH}$	3.2
glutamine	Gln	$\text{H}_2\text{N}-\underset{\text{CH}_2-\text{CH}_2-\underset{\text{O}}{\underset{\parallel}{\text{C}}}-\text{NH}_2}{\underset{\text{CH}_2}{\text{CH}}}-\text{COOH}$	5.7
glycine	Gly	$\text{H}_2\text{N}-\text{CH}_2-\text{COOH}$	6.0
histidine	His	$\text{H}_2\text{N}-\underset{\text{CH}_2}{\underset{\text{CH}_2}{\text{CH}}}-\text{COOH}$ 	7.6
isoleucine	Ile	$\text{H}_2\text{N}-\underset{\text{H}_3\text{C}-\text{CH}}{\underset{\text{CH}_2-\text{CH}_2-\text{CH}_3}{\text{CH}}}-\text{COOH}$	6.0
leucine	Leu	$\text{H}_2\text{N}-\underset{\text{H}_3\text{C}-\text{CH}}{\underset{\text{CH}_2}{\text{CH}}}-\text{COOH}$	6.0
lysine	Lys	$\text{H}_2\text{N}-\underset{\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{NH}_2}{\underset{\text{CH}_2}{\text{CH}}}-\text{COOH}$	9.7

Common name	Symbol	Structural formula	pH of isoelectric point
methionine	Met	$\text{H}_2\text{N}-\underset{\text{CH}_2-\text{CH}_2-\text{S}-\text{CH}_3}{\text{CH}}-\text{COOH}$	5.7
phenylalanine	Phe	$\text{H}_2\text{N}-\underset{\text{CH}_2}{\text{CH}}-\text{COOH}$ 	5.5
proline	Pro		6.3
serine	Ser	$\text{H}_2\text{N}-\underset{\text{CH}_2-\text{OH}}{\text{CH}}-\text{COOH}$	5.7
threonine	Thr	$\text{H}_2\text{N}-\underset{\text{H}_3\text{C}-\text{CH}-\text{OH}}{\text{CH}}-\text{COOH}$	5.6
tryptophan	Trp	$\text{H}_2\text{N}-\underset{\text{CH}_2}{\text{CH}}-\text{COOH}$ 	5.9
tyrosine	Tyr		5.7
valine	Val	$\text{H}_2\text{N}-\underset{\text{H}_3\text{C}-\text{CH}-\text{CH}_3}{\text{CH}}-\text{COOH}$	6.0

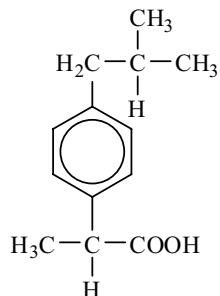
## 20. Structural formulas of some medicines and drugs



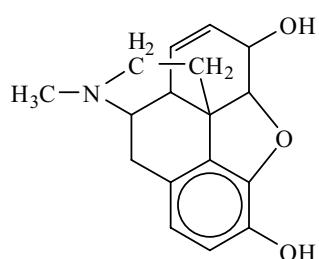
aspirin



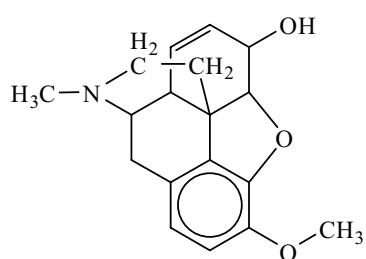
paracetamol (acetaminophen)



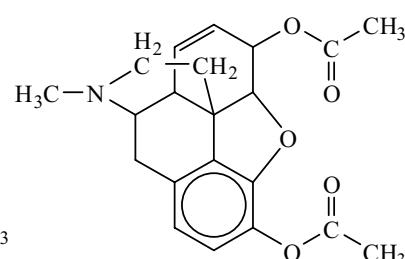
ibuprofen



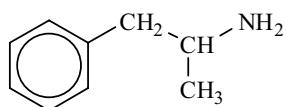
morphine



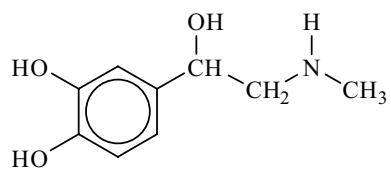
codeine



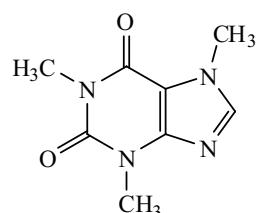
diamorphine (heroin)



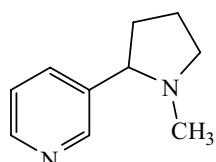
amphetamine



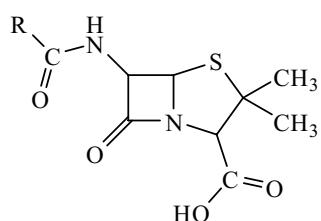
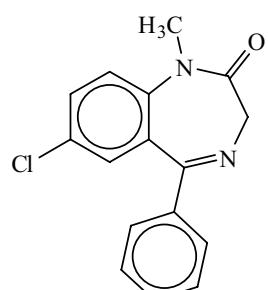
epinephrine (adrenaline)



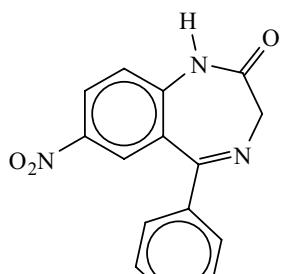
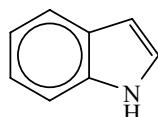
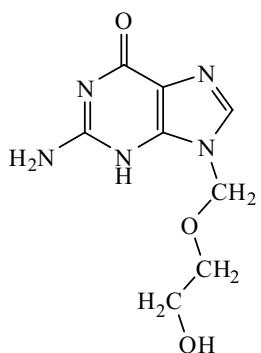
caffeine



nicotine

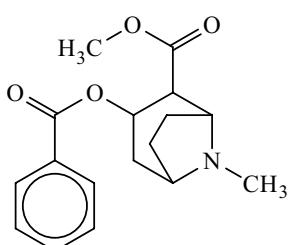
penicillin  
(general structure)

diazepam (Valium®)

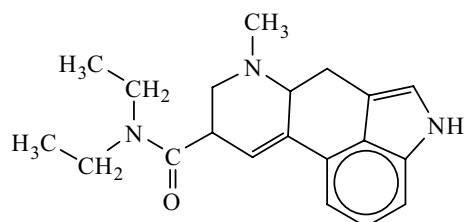
nitrazepam (Mogadon<sup>®</sup>)

indole

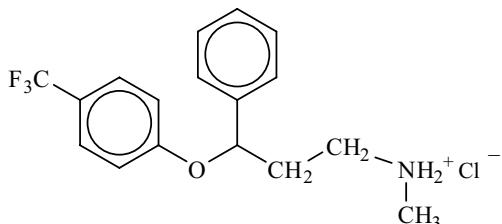
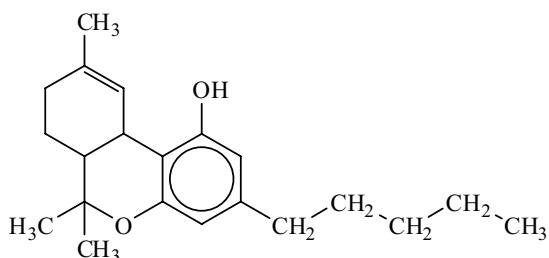
acyclovir



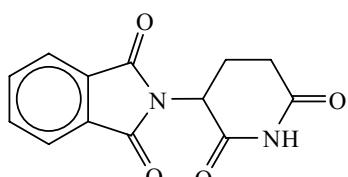
cocaine



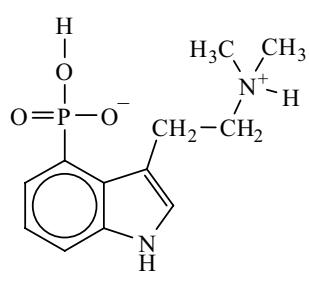
lysergic acid diethylamide (LSD)

fluoxetine hydrochloride (Prozac<sup>®</sup>)

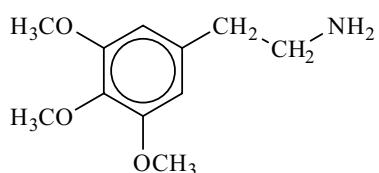
tetrahydrocannabinol (THC)



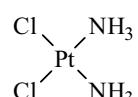
thalidomide



psilocybin

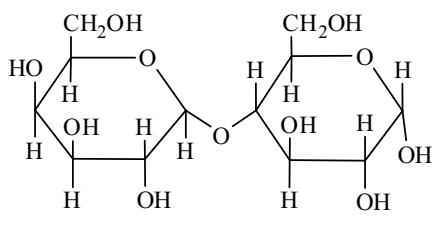


mescaline

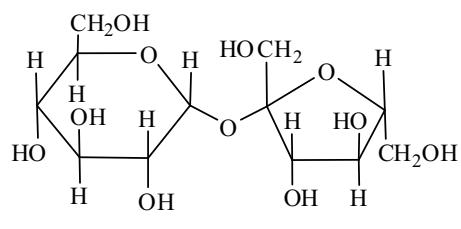


cisplatin

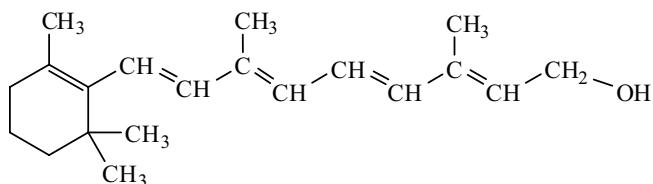
## 21. Structural formulas of some biological molecules



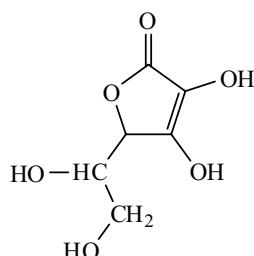
lactose



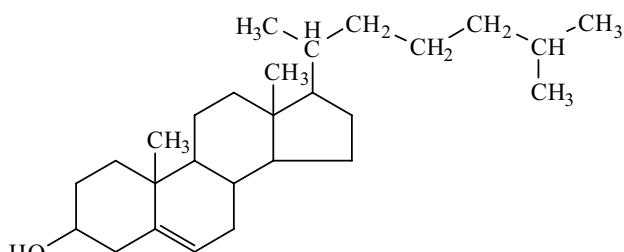
sucrose



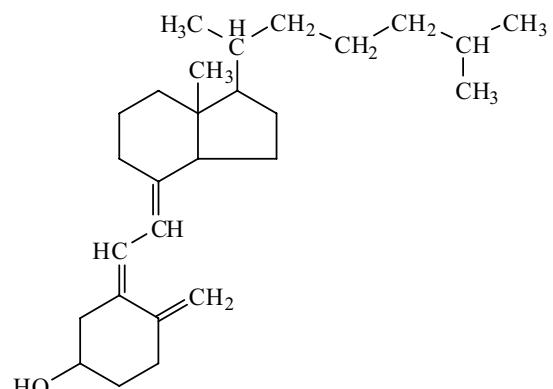
retinol (vitamin A)



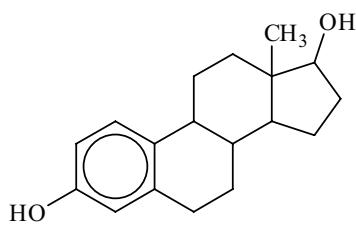
ascorbic acid (vitamin C)



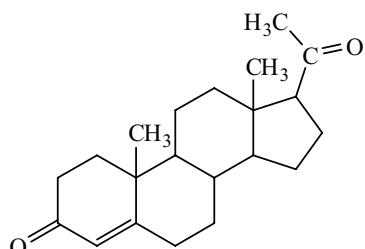
cholesterol



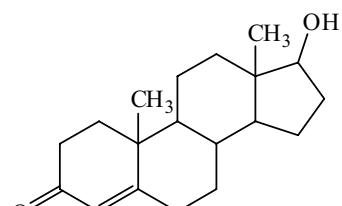
vitamin D



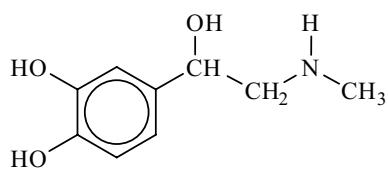
estradiol



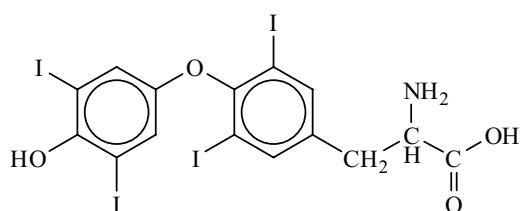
progesterone



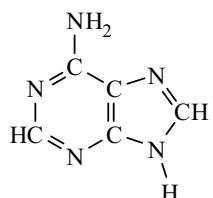
testosterone



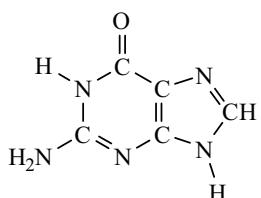
epinephrine (adrenaline)



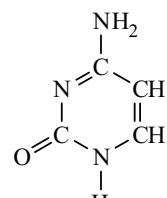
thyroxine



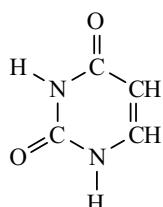
adenine



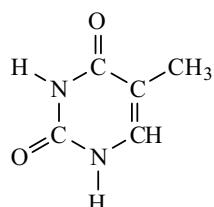
guanine



cytosine



uracil

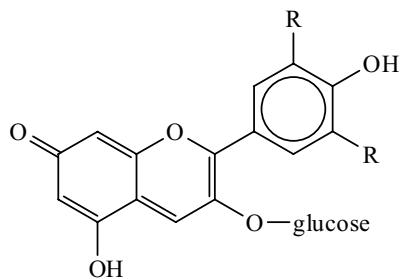


thymine

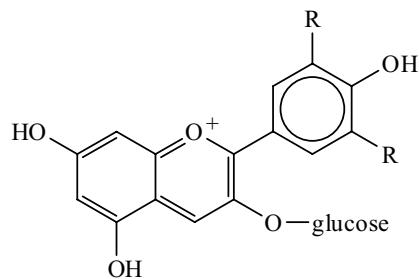
## 22. Structural formulas of some food chemistry molecules

### Natural pigments

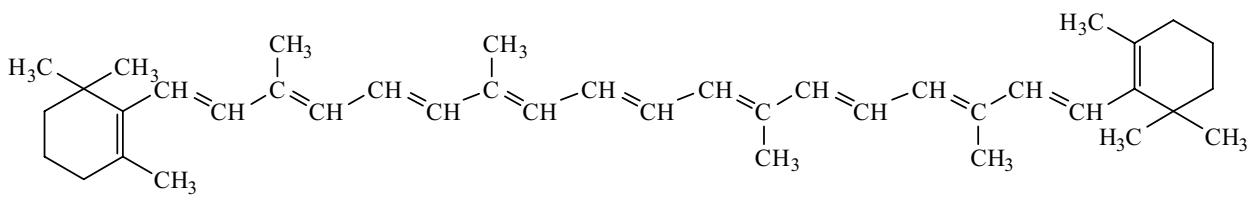
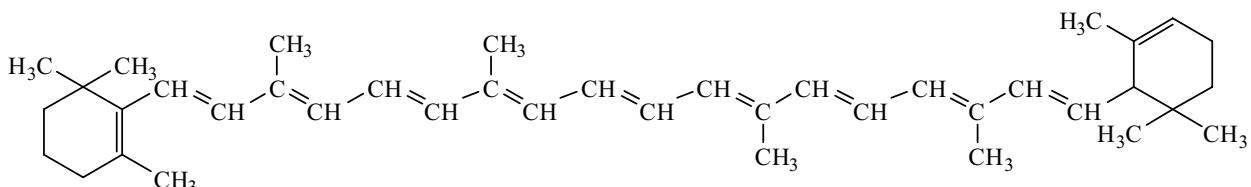
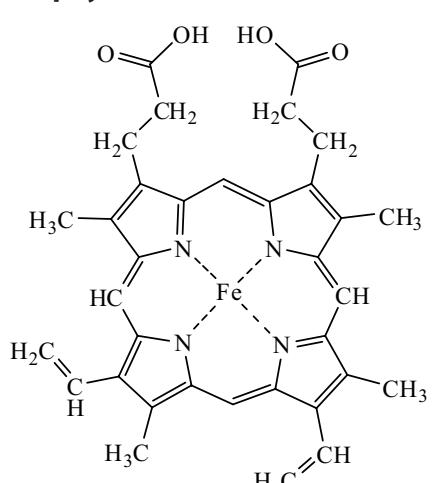
#### Anthocyanins



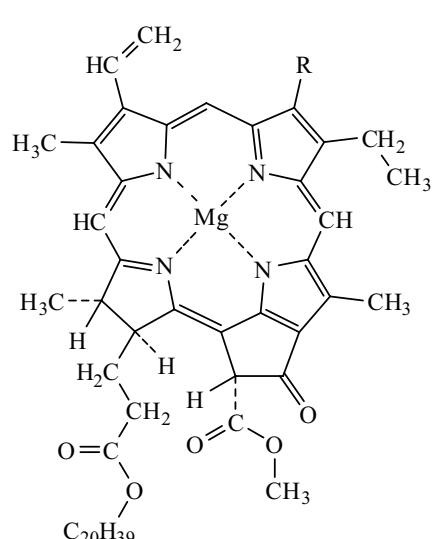
quinoidal base (blue)



flavylium cation (red)

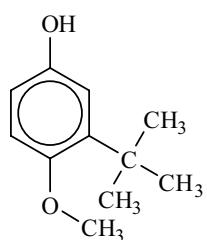
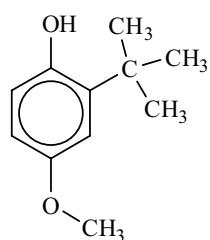
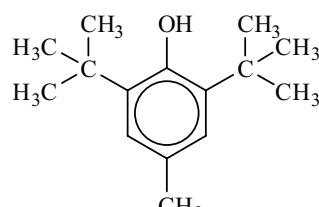
**Carotenes****Porphyrins**

heme B



chlorophyll

R=CH<sub>3</sub> (Chlorophyll a)  
R=CHO (Chlorophyll b)

**Preservatives**2-*tert*-butyl-4-hydroxyanisole  
(2-BHA)3-*tert*-butyl-4-hydroxyanisole (3-BHA)3,5-di-*tert*-butyl-4-hydroxytoluene (BHT)

## Fatty acids

Fatty acid	Formula
Octanoic acid	$\text{CH}_3(\text{CH}_2)_6\text{COOH}$
Lauric acid	$\text{CH}_3(\text{CH}_2)_{10}\text{COOH}$
Stearic acid	$\text{CH}_3(\text{CH}_2)_{16}\text{COOH}$
Oleic acid	$\text{CH}_3(\text{CH}_2)\text{-CH=CH}(\text{CH}_2)\text{-COOH}$
Linoleic acid	$\text{CH}_3(\text{CH}_2)_4(\text{CH=CHCH}_2)_2(\text{CH}_2)_6\text{COOH}$
Linolenic acid	$\text{CH}_3\text{CH}_2(\text{CH=CHCH}_2)_3(\text{CH}_2)_6\text{COOH}$

## 23. References

The data in tables 4–16 can be found in the following three sources.

Lide, DR. 2008. *CRC Handbook of Chemistry and Physics*. Boca Raton, USA. CRC Press. Copyright 2008 by *CRC Handbook of Chemistry and Physics*. David R Lide. Reproduced by permission from Taylor and Francis Group, LLC, a division of Informa plc.

NVON. 2007. *Binas*. English Edition. Groningen, The Netherlands. Wolters-Noordhoff.

Royal Society of Chemistry. 2002. *Royal Society of Chemistry Electronic Data Book CD-Rom*. London, UK. Reproduced by permission of The Royal Society of Chemistry.

For tables 17 and 18, in addition to the sources above, the data were informed by the following.

Aylward, G and Findlay, T. 2002. *SI Chemical Data*. 5th Edition. Queensland, Australia. John Wiley & Sons.

Clugston, M and Flemming, R. 2000. *Advanced Chemistry*. Oxford, UK. Oxford University Press.

Morrison, RT and Boyd, RN. 1987. *Organic Chemistry*. 5th Edition. Boston, Massachusetts, USA. Allyn and Bacon, Inc.