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# Chemistry data booklet

First examinations 2009



## **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 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

$$\log_{10} \frac{I_0}{I} = \epsilon l c$$

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

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

$$c = f \lambda$$

$$PV = nRT$$

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

$$q = mc \Delta T$$

$$E = hf$$

## 2. Physical constants and unit conversions

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

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

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

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

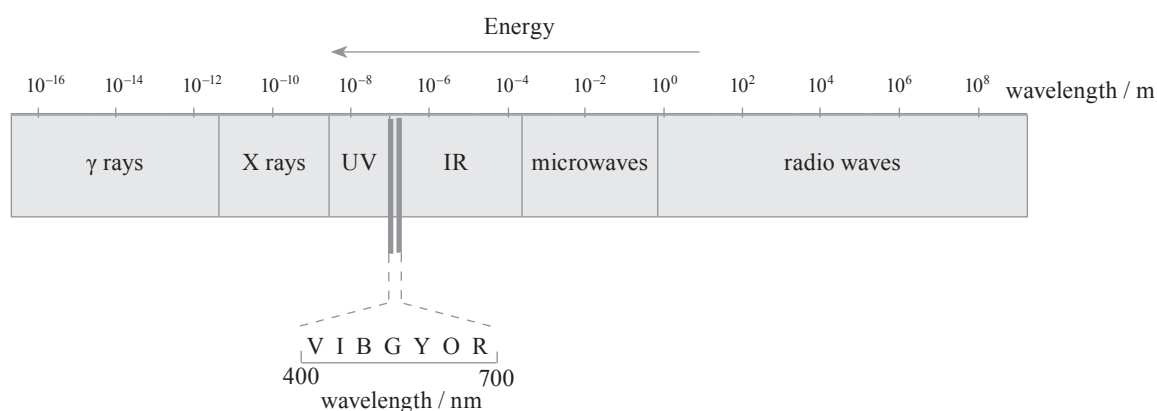
Specific heat capacity of water =  $4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$  (=  $4.18 \text{ J g}^{-1} \text{ K}^{-1}$ )

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

1 atm =  $1.01 \times 10^5 \text{ Pa}$

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

## 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			







## 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	<b>H</b>	-73							2372	<b>He</b>										
520	<b>Li</b>	-60	900						2081	<b>Ne</b>										
		1.0	1.6							<b>F</b>										
										4.0										
496	<b>Na</b>	-53	738							<b>O</b>										
		0.9	1.3							1314 -141 +798										
										3.4										
										<b>N</b>										
										1402										
										3.0										
										<b>C</b>										
										1086 -122										
										2.6										
										<b>B</b>										
										801 -27										
										2.0										
										<b>Al</b>										
										578 -42										
										1.6										
										<b>Si</b>										
										789 -134										
										1.9										
										<b>P</b>										
										1012 -72										
										2.2										
										<b>S</b>										
										1000 -200 +640										
										2.6										
										<b>Cl</b>										
										1251 -349										
										3.2										
										<b>Ar</b>										
										1521										
419	<b>K</b>	-48	590	-2	631 -18	658 -8	650 -51	653 -64	717	759 -15	758 -64	737 -112	746 -119	906	579 -41	762 -119	947 -79	941 -195	1140 -325	1351
		0.8	1.0	1.0	1.4	1.5	1.6	1.7	1.6	1.8	1.9	1.9	1.9	1.7	1.8	2.0	2.2	2.6	3.0	<b>Kr</b>
																				<b>Ga</b>
																				<b>Br</b>
																				<b>Se</b>
																				<b>As</b>
																				<b>Sb</b>
																				<b>Te</b>
																				<b>I</b>
																				<b>At</b>
																				<b>Po</b>
																				<b>Rn</b>
																				<b>Bi</b>
																				<b>Pb</b>
																				<b>Tl</b>
																				<b>Hg</b>
																				<b>Au</b>
																				<b>Pt</b>
																				<b>Ir</b>
																				<b>Os</b>
																				<b>Re</b>
																				<b>W</b>
																				<b>Ta</b>
																				<b>Hf</b>
																				<b>La</b>
																				<b>Ba</b>
																				<b>Ra</b>
																				<b>Ac</b>
393	<b>Fr</b>	-46	503	-14	538 -45	680	761 -31	770 -79	760 -14	840 -106	880 -151	870 -205	890 -223	1007	589 -19	716 -35	703 -91	812 -183	-270	1037
		0.7	0.9	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	<b>Rn</b>
																				<b>At</b>
																				<b>Po</b>
																				<b>Bi</b>
																				<b>Pb</b>
																				<b>Tl</b>
																				<b>Hg</b>
																				<b>Au</b>
																				<b>Pt</b>
																				<b>Ir</b>
																				<b>Os</b>
																				<b>Re</b>
																				<b>W</b>
																				<b>Ta</b>
																				<b>Hf</b>
																				<b>La</b>
																				<b>Ba</b>
																				<b>Ra</b>
																				<b>Ac</b>

## 8. Atomic and ionic radii of the elements

		Element																He			
		Ionic radius / $10^{-12}$ m								Atomic radius / $10^{-12}$ m											
30	<b>H</b>																				
152	<b>Be</b>	112																64	<b>Ne</b>		
68 (1+)	<b>Li</b>	30 (2+)																66	<b>O</b>		
186	<b>Na</b>	160																70	<b>N</b>		
98 (1+)	<b>Mg</b>	65 (2+)																77	<b>C</b>		
231	<b>K</b>	197	160	146	131	125	129	126	125	124	128	133	141	143	144	141	122	121	117	114	<b>Kr</b>
133 (1+)	<b>Ca</b>	81 (3+)	81 (3+)	90 (2+) 68 (4+)	88 (2+)	88 (2+)	80 (2+) 60 (4+)	76 (2+) 64 (3+)	74 (2+) 63 (3+)	72 (2+)	69 (2+)	74 (2+)	62 (3+)	53 (4+) 272 (4+)	42 (4+) 271 (4+)	212 (3-)	190 (2-)	202 (2-)	196 (1-)	196 (1-)	<b>Br</b>
244	<b>Rb</b>	215	180	157	141	136	135	133	134	138	144	149	166	162	162	141	137	137	133	133	<b>Xe</b>
148 (1+)	<b>Sr</b>	110 (2+)	93 (3+)	80 (4+)	64 (5+)	64 (4+)	65 (4+) 37 (7+)	68 (3+) 62 (4+)	67 (3+) 60 (4+)	86 (2+) 62 (4+)	126 (1+)	97 (2+)	81 (3+)	112 (2+) 71 (4+)	245 (3-)	222 (2-)	222 (2-)	219 (1-)	219 (1-)	219 (1-)	<b>I</b>
262	<b>Cs</b>	217	188	157	143	137	137	134	134	138	144	152	171	175	170	170	140	140	140	140	<b>Rn</b>
167 (1+)	<b>Ba</b>	134 (2+)	115 (3+)	76 (4+)	72 (6+)	66 (4+)	63 (4+) 38 (7+)	63 (4+) 39 (8+)	68 (3+) 63 (4+)	80 (2+) 63 (4+)	85 (3+)	110 (2+)	93 (3+)	120 (2+) 84 (4+)	120 (3+) 76 (5+)	94 (4+) 67 (6+)	62 (7+)	62 (7+)	62 (7+)	62 (7+)	<b>At</b>
270	<b>Fr</b>	180 (1+)	148 (2+)	112 (3+)	188	220	188	188	188	188	188	188	188	188	188	188	188	188	188	188	<b>Ra</b>
180 (1+)	<b>Ac</b>	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	112 (3+)	<b>Ac</b>

## 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	C-O	358
O=O	498	C=O	746
S-S	266	C-N	286
F-F	158	C=N	615
Cl-Cl	243	C≡N	887
Br-Br	193	C-F	467
I-I	151	C-Cl	346
		C-Br	290
		C-I	228
		Si-O	466

## 11. Organic compounds—thermodynamic data

Substance	Formula	State	$\Delta H_f^\ominus /$ kJ mol <sup>-1</sup>	$\Delta G_f^\ominus /$ kJ mol <sup>-1</sup>	$S^\ominus /$ J K <sup>-1</sup> mol <sup>-1</sup>
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	$\Delta H_c^\ominus / \text{kJ mol}^{-1}$	Substance	Formula	State	$\Delta H_c^\ominus / \text{kJ mol}^{-1}$
hydrogen	H <sub>2</sub>	g	-286	propan-1-ol	C <sub>3</sub> H <sub>7</sub> OH	l	-2021
sulfur	S	s	-297	butan-1-ol	C <sub>4</sub> H <sub>9</sub> OH	l	-2676
carbon (graphite)	C	s	-394	cyclohexanol	C <sub>6</sub> H <sub>11</sub> OH	s	-3727
carbon monoxide	CO	g	-283	phenol	C <sub>6</sub> H <sub>5</sub> OH	s	-3053
methane	CH <sub>4</sub>	g	-890	ethoxyethane	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	l	-2724
ethane	C <sub>2</sub> H <sub>6</sub>	g	-1560	methanal	HCHO	g	-571
propane	C <sub>3</sub> H <sub>8</sub>	g	-2219	ethanal	CH <sub>3</sub> CHO	g	-1167
butane	C <sub>4</sub> H <sub>10</sub>	g	-2877	benzaldehyde	C <sub>6</sub> H <sub>5</sub> CHO	l	-3525
pentane	C <sub>5</sub> H <sub>12</sub>	l	-3509	propanone	(CH <sub>3</sub> ) <sub>2</sub> CO	l	-1817
hexane	C <sub>6</sub> H <sub>14</sub>	l	-4163	pentan-3-one	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	l	-3100
octane	C <sub>8</sub> H <sub>18</sub>	l	-5470	phenylethanone	CH <sub>3</sub> COC <sub>6</sub> H <sub>5</sub>	l	-4149
cyclohexane	C <sub>6</sub> H <sub>12</sub>	l	-3920	methanoic acid	HCOOH	l	-254
ethene	C <sub>2</sub> H <sub>4</sub>	g	-1411	ethanoic acid	CH <sub>3</sub> COOH	l	-874
buta-1,3-diene	C <sub>4</sub> H <sub>6</sub>	g	-2541	benzoic acid	C <sub>6</sub> H <sub>5</sub> COOH	s	-3227
ethyne	C <sub>2</sub> H <sub>2</sub>	g	-1301	ethanedioic acid	(COOH) <sub>2</sub>	s	-243
benzene	C <sub>6</sub> H <sub>6</sub>	l	-3267	ethyl ethanoate	CH <sub>3</sub> COOC <sub>2</sub> H <sub>5</sub>	l	-2238
methylbenzene	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	l	-3910	ethanamide	CH <sub>3</sub> CONH <sub>2</sub>	s	-1185
naphthalene	C <sub>10</sub> H <sub>8</sub>	s	-5156	methylamine	CH <sub>3</sub> NH <sub>2</sub>	g	-1085
chloroethane	C <sub>2</sub> H <sub>5</sub> Cl	g	-1413	ethylamine	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	g	-1740
bromoethane	C <sub>2</sub> H <sub>5</sub> Br	l	-1425	phenylamine	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	l	-3393
iodoethane	C <sub>2</sub> H <sub>5</sub> I	l	-1467	nitrobenzene	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	l	-3088
(chloromethyl)benzene	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> Cl	l	-3709	urea	CO(NH <sub>2</sub> ) <sub>2</sub>	s	-632
trichloromethane	CHCl <sub>3</sub>	l	-474	glucose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	s	-2803
methanol	CH <sub>3</sub> OH	l	-726	sucrose	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	s	-5640
ethanol	C <sub>2</sub> H <sub>5</sub> OH	l	-1367				

## 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	$\rightleftharpoons$	Reduced species	$E^\ominus / \text{V}$
$\text{Li}^+(\text{aq}) + \text{e}^-$	$\rightleftharpoons$	$\text{Li}(\text{s})$	-3.04
$\text{K}^+(\text{aq}) + \text{e}^-$	$\rightleftharpoons$	$\text{K}(\text{s})$	-2.93
$\text{Ca}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Ca}(\text{s})$	-2.87
$\text{Na}^+(\text{aq}) + \text{e}^-$	$\rightleftharpoons$	$\text{Na}(\text{s})$	-2.71
$\text{Mg}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Mg}(\text{s})$	-2.37
$\text{Al}^{3+}(\text{aq}) + 3\text{e}^-$	$\rightleftharpoons$	$\text{Al}(\text{s})$	-1.66
$\text{Mn}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Mn}(\text{s})$	-1.19
$\text{H}_2\text{O}(\text{l}) + \text{e}^-$	$\rightleftharpoons$	$\frac{1}{2}\text{H}_2(\text{g}) + \text{OH}^-(\text{aq})$	-0.83
$\text{Zn}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Zn}(\text{s})$	-0.76
$\text{Fe}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Fe}(\text{s})$	-0.45
$\text{Ni}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Ni}(\text{s})$	-0.26
$\text{Sn}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Sn}(\text{s})$	-0.14
$\text{Pb}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Pb}(\text{s})$	-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
$\text{SO}_4^{2-}(\text{aq}) + 4\text{H}^+(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{H}_2\text{SO}_3(\text{aq}) + \text{H}_2\text{O}(\text{l})$	+0.17
$\text{Cu}^{2+}(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{Cu}(\text{s})$	+0.34
$\frac{1}{2}\text{O}_2(\text{g}) + \text{H}_2\text{O}(\text{l}) + 2\text{e}^-$	$\rightleftharpoons$	$2\text{OH}^-(\text{aq})$	+0.40
$\text{Cu}^+(\text{aq}) + \text{e}^-$	$\rightleftharpoons$	$\text{Cu}(\text{s})$	+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
$\text{Ag}^+(\text{aq}) + \text{e}^-$	$\rightleftharpoons$	$\text{Ag}(\text{s})$	+0.80
$\frac{1}{2}\text{Br}_2(\text{l}) + \text{e}^-$	$\rightleftharpoons$	$\text{Br}^-(\text{aq})$	+1.07
$\frac{1}{2}\text{O}_2(\text{g}) + 2\text{H}^+(\text{aq}) + 2\text{e}^-$	$\rightleftharpoons$	$\text{H}_2\text{O}(\text{l})$	+1.23
$\text{Cr}_2\text{O}_7^{2-}(\text{aq}) + 14\text{H}^+(\text{aq}) + 6\text{e}^-$	$\rightleftharpoons$	$2\text{Cr}^{3+}(\text{aq}) + 7\text{H}_2\text{O}(\text{l})$	+1.33
$\frac{1}{2}\text{Cl}_2(\text{g}) + \text{e}^-$	$\rightleftharpoons$	$\text{Cl}^-(\text{aq})$	+1.36
$\text{MnO}_4^-(\text{aq}) + 8\text{H}^+(\text{aq}) + 5\text{e}^-$	$\rightleftharpoons$	$\text{Mn}^{2+}(\text{aq}) + 4\text{H}_2\text{O}(\text{l})$	+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> ICOOH	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> 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 <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	p <i>K</i> <sub>a</sub>
methanol	CH <sub>3</sub> OH	15.5
ethanol	C <sub>2</sub> H <sub>5</sub> OH	15.5

## Amines

Name	Formula	p <i>K</i> <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 <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	p <i>K</i> <sub>a</sub>	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 / $\text{cm}^{-1}$
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

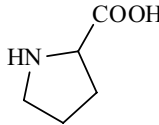
Typical proton chemical shift values ( $\delta$ ) relative to tetramethylsilane (TMS) = 0.

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

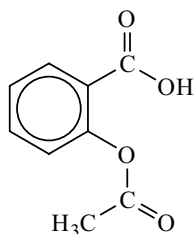
These values may vary in different solvents and conditions.

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
$\text{—C}\equiv\text{C—H}$	1.8–3.1
$\text{—CH}_2\text{—Hal}$	3.5–4.4
$\text{R—O—CH}_2\text{—}$	3.3–3.7
	3.8–4.1
	9.0–13.0
$\text{R—O—H}$	4.0–12.0
$\text{—HC=CH}_2$	4.5–6.0
	4.0–12.0
	6.9–9.0
	9.4–10.0

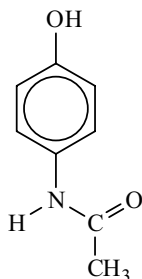


Common name	Symbol	Structural formula	pH of isoelectric point
methionine	Met	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\   \\ \text{CH}_2-\text{CH}_2-\text{S}-\text{CH}_3 \end{array}$	5.7
phenylalanine	Phe	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\   \\ \text{CH}_2 \\   \\ \text{C}_6\text{H}_5 \end{array}$	5.5
proline	Pro		6.3
serine	Ser	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\   \\ \text{CH}_2-\text{OH} \end{array}$	5.7
threonine	Thr	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\   \\ \text{H}_3\text{C}-\text{CH}-\text{OH} \end{array}$	5.6
tryptophan	Trp	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\   \\ \text{CH}_2 \\   \\ \text{C}_8\text{H}_6\text{N}_2 \end{array}$	5.9
tyrosine	Tyr	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\   \\ \text{CH}_2 \\   \\ \text{C}_6\text{H}_4 \\   \\ \text{OH} \end{array}$	5.7
valine	Val	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\   \\ \text{H}_3\text{C}-\text{CH}-\text{CH}_3 \end{array}$	6.0

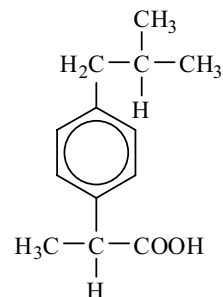
## 20. Structural formulas of some medicines and drugs



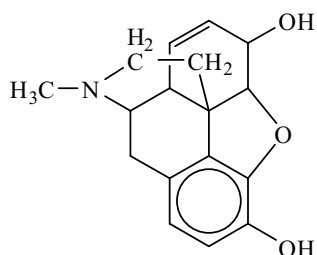
aspirin



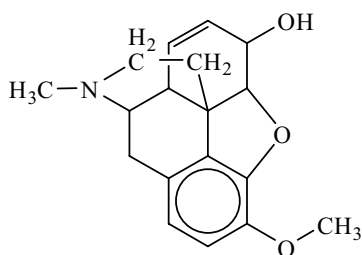
paracetamol (acetaminophen)



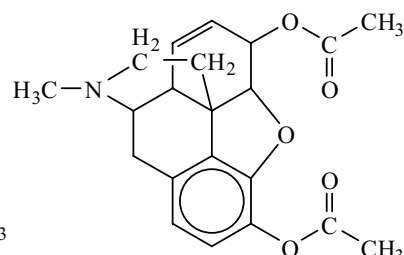
ibuprofen



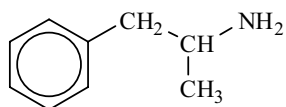
morphine



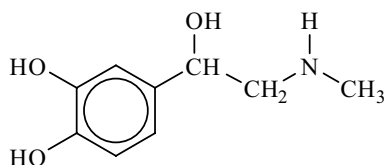
codeine



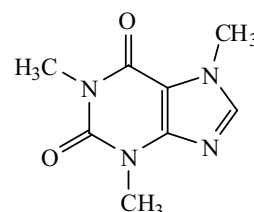
diamorphine (heroin)



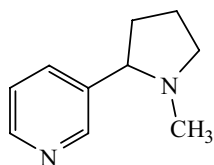
amphetamine



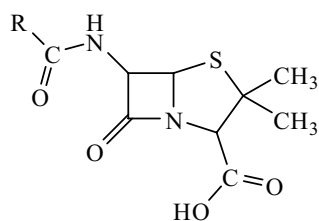
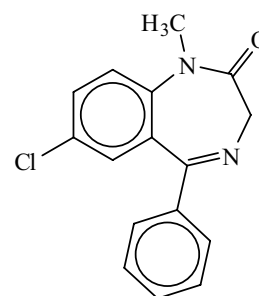
epinephrine (adrenaline)



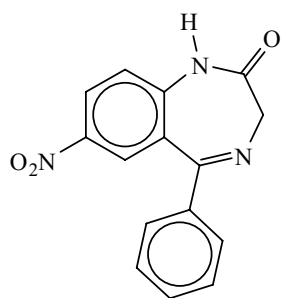
caffeine



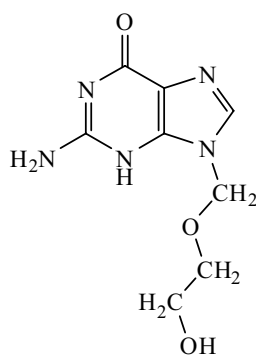
nicotine

penicillin  
(general structure)

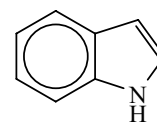
diazepam (Valium®)



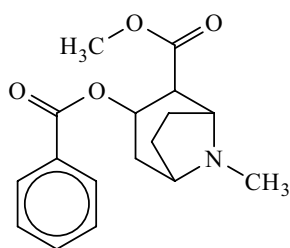
nitrazepam (Mogadon®)



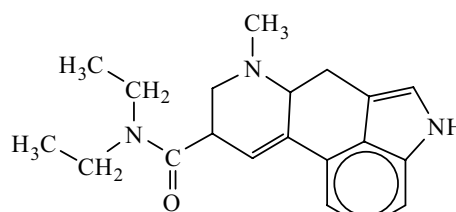
acyclovir



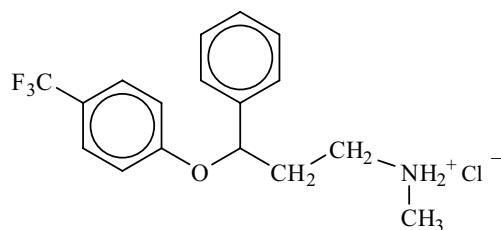
indole



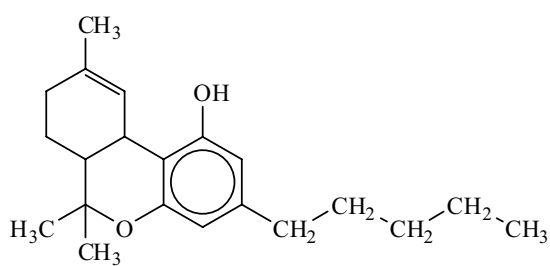
cocaine



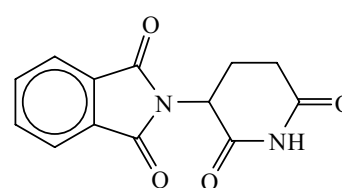
lysergic acid diethylamide (LSD)



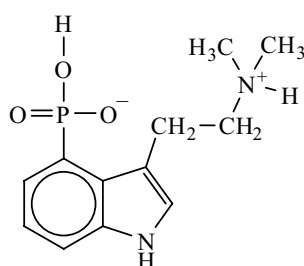
fluoxetine hydrochloride (Prozac®)



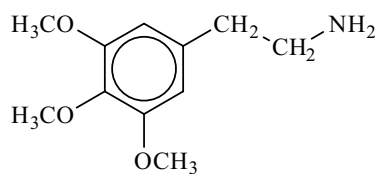
tetrahydrocannabinol (THC)



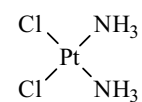
thalidomide



psilocybin



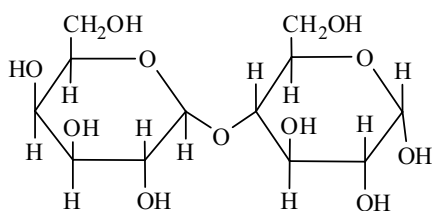
mescaline



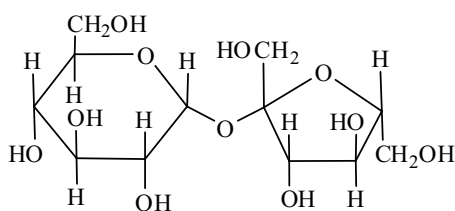
cisplatin



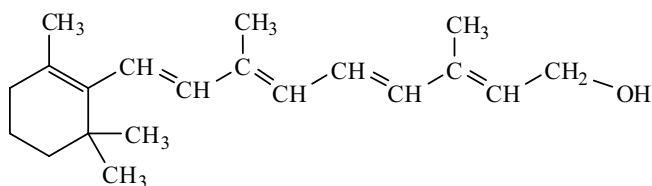
## 21. Structural formulas of some biological molecules



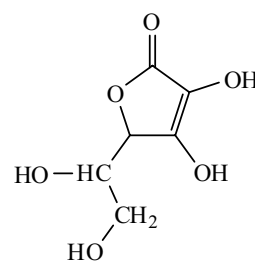
lactose



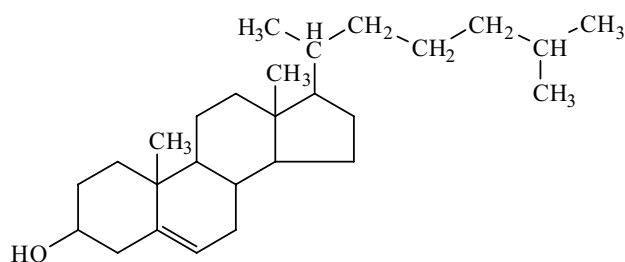
sucrose



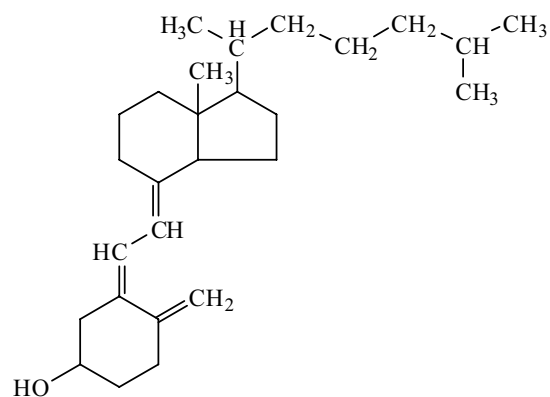
retinol (vitamin A)



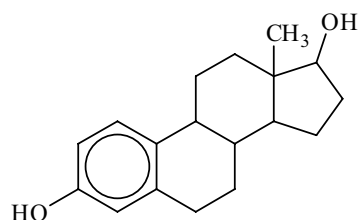
ascorbic acid (vitamin C)



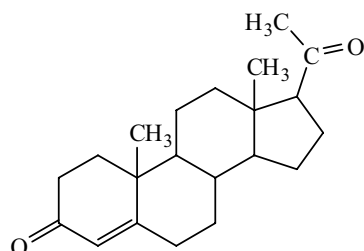
cholesterol



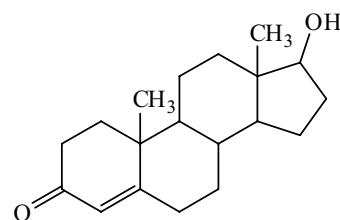
vitamin D



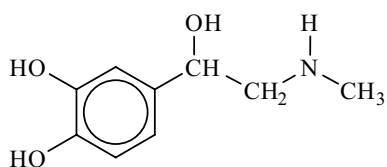
estradiol



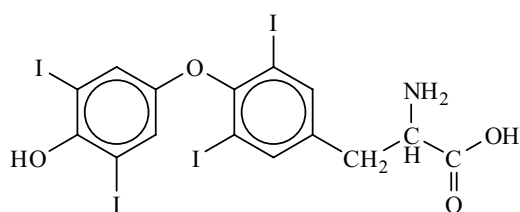
progesterone



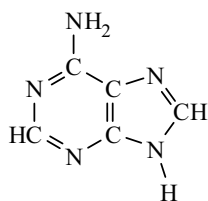
testosterone



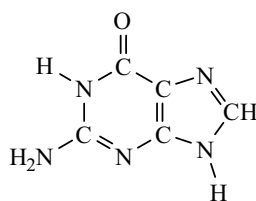
epinephrine (adrenaline)



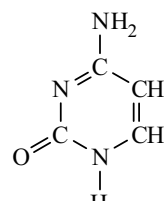
thyroxine



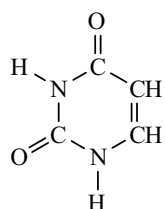
adenine



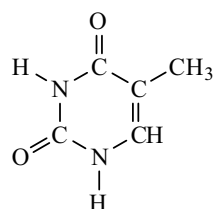
guanine



cytosine



uracil

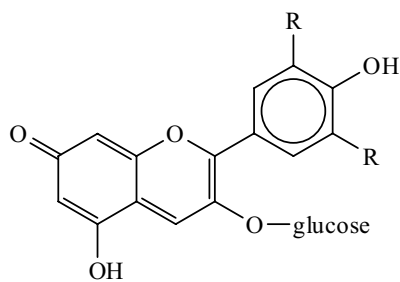


thymine

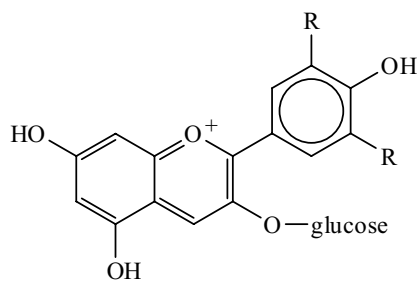
## 22. Structural formulas of some food chemistry molecules

### Natural pigments

#### Anthocyanins

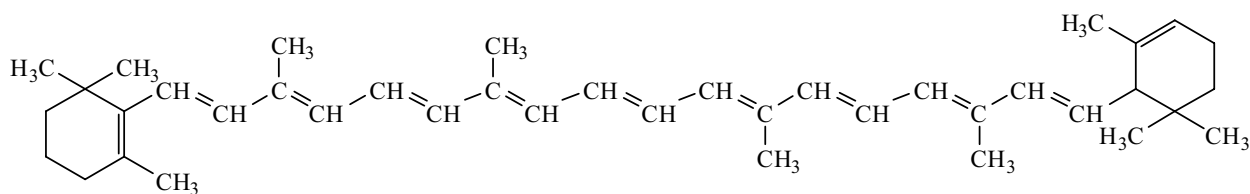
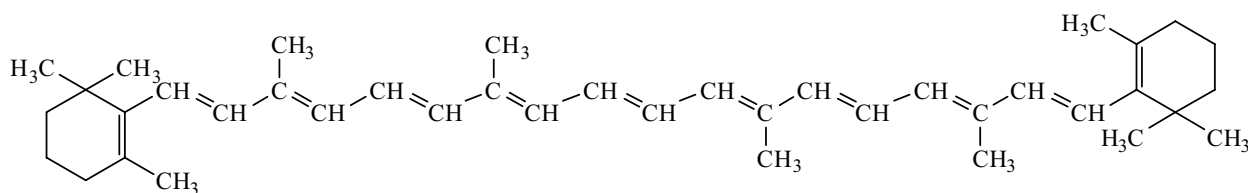


quinoidal base (blue)

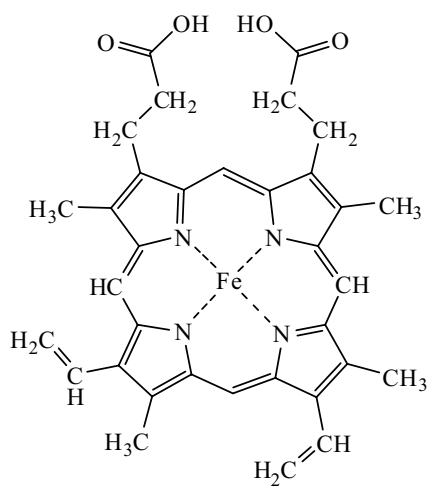


flavylium cation (red)

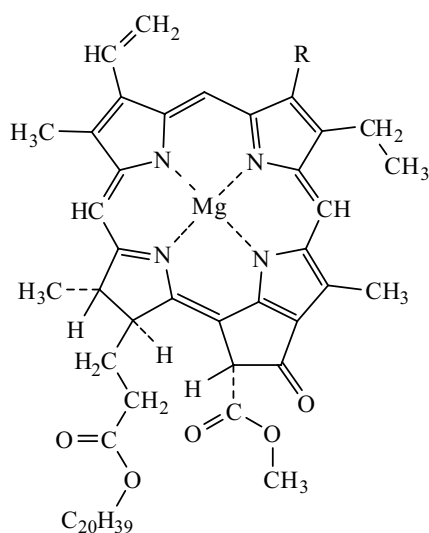
## Carotenes

 $\alpha$ -carotene $\beta$ -carotene

## Porphyrins



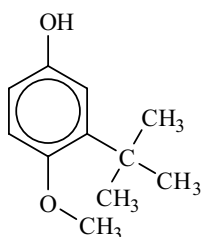
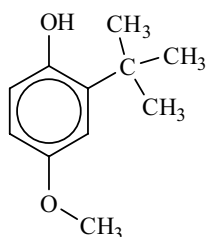
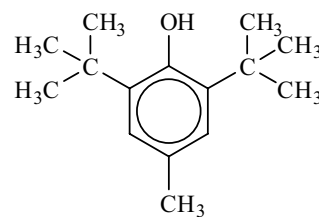
heme B



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

chlorophyll

## 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	$\text{CH}_3(\text{CH}_2)_7\text{CH}=\text{CH}(\text{CH}_2)_7\text{COOH}$
Linoleic acid	$\text{CH}_3(\text{CH}_2)_4(\text{CH}=\text{CHCH}_2)_2(\text{CH}_2)_6\text{COOH}$
Linolenic acid	$\text{CH}_3\text{CH}_2(\text{CH}=\text{CHCH}_2)_3(\text{CH}_2)_6\text{COOH}$

## 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.

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

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