

Chemistry
First examinations 2009

Diploma Programme

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 4 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).

I. Some relevant equations

$$t_{\frac{1}{2}} = \frac{0.693}{k}$$

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

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

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

$$E = hf$$

$$PV = nRT$$

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

2. Physical constants

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

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

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

Planck's constant (h) = 6.63×10^{-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) = 1.00×10^{-14} mol 2 dm $^{-6}$ at 298 K

1 atm = 1.01×10^5 Pa

1 dm 3 = 1 litre = 1×10^{-3} m 3 = 1×10^3 cm 3

3. Fundamental particles

	Proton	Neutron	Electron
Mass (kg)	1.672648×10^{-27}	1.674954×10^{-27}	9.109534×10^{-31}
Charge (C)	1.602189×10^{-19}	0	1.602189×10^{-19}

4. Names of the first 103 elements

Element	Symbol	Atomic number	Element	Symbol	Atomic number
actinium	Ac	89	fluorine	F	9
aluminium	Al	13	francium	Fr	87
americium	Am	95	gadolinium	Gd	64
antimony	Sb	51	gallium	Ga	31
argon	Ar	18	germanium	Ge	32
arsenic	As	33	gold	Au	79
astatine	At	85	hafnium	Hf	72
barium	Ba	56	helium	He	2
berkelium	Bk	97	holmium	Ho	67
beryllium	Be	4	hydrogen	H	1
bismuth	Bi	83	indium	In	49
boron	B	5	iodine	I	53
bromine	Br	35	iridium	Ir	77
cadmium	Cd	48	iron	Fe	26
caesium	Cs	55	krypton	Kr	36
calcium	Ca	20	lanthanum	La	57
californium	Cf	98	lawrencium	Lr	103
carbon	C	6	lead	Pb	82
cerium	Ce	58	lithium	Li	3
chlorine	Cl	17	lutetium	Lu	71
chromium	Cr	24	magnesium	Mg	12
cobalt	Co	27	manganese	Mn	25
copper	Cu	29	mendelevium	Md	101
curium	Cm	96	mercury	Hg	80
dysprosium	Dy	66	molybdenum	Mo	42
einsteinium	Es	99	neodymium	Nd	60
erbium	Er	68	neon	Ne	10
europium	Eu	63	neptunium	Np	93
fermium	Fm	100	nickel	Ni	28

Element	Symbol	Atomic number	Element	Symbol	Atomic number
niobium	Nb	41	silicon	Si	14
nitrogen	N	7	silver	Ag	47
nobelium	No	102	sodium	Na	11
osmium	Os	76	strontium	Sr	38
oxygen	O	8	sulfur	S	16
palladium	Pd	46	tantalum	Ta	73
phosphorus	P	15	technetium	Tc	43
platinum	Pt	78	tellurium	Te	52
plutonium	Pu	94	terbium	Tb	65
polonium	Po	84	thallium	Tl	81
potassium	K	19	thorium	Th	90
praseodymium	Pr	59	thulium	Tm	69
promethium	Pm	61	tin	Sn	50
protactinium	Pa	91	titanium	Ti	22
radium	Ra	88	tungsten	W	74
radon	Rn	86	uranium	U	92
rhenium	Re	75	vanadium	V	23
rhodium	Rh	45	xenon	Xe	54
rubidium	Rb	37	ytterbium	Yb	70
ruthenium	Ru	44	yttrium	Y	39
samarium	Sm	62	zinc	Zn	30
scandium	Sc	21	zirconium	Zr	40
selenium	Se	34			

5. The periodic table

1	2													3	4	5	6	7	0	
1 H 1.01	4 Be 9.01													2 He 4.00						
		Atomic number Element																		
11 Na 22.99	12 Mg 24.31	20 Ca 40.08	21 Sc 44.96	22 Ti 47.90	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.71	29 Cu 63.55	30 Zn 65.37	31 Ga 69.72	32 Ge 72.59	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80		
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc 98.91	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.40	49 In 114.82	50 Sn 118.69	51 Sb 121.75	52 Te 127.60	53 I 126.90	54 Xe 131.30			
55 Cs 132.91	56 Ba 137.34	57 † La 138.91	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.21	76 Os 190.21	77 Ir 192.22	78 Pt 195.09	79 Au 196.97	80 Hg 200.59	81 Tl 204.37	82 Pb 207.19	83 Bi 208.98	84 Po (210)	85 At (210)	86 Rn (222)			
87 Fr (223)	88 Ra (226)	89 ‡ Ac (227)																		
†		58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm 146.92	62 Sm 150.35	63 Eu 151.96	64 Gd 157.25	65 Tb 158.92	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 (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (254)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (260)					

6. Melting points and boiling points of the elements

14 H 20	Melting point (K) Element Boiling point (K)												1 He 4					
454 Li 1600	1551 Be 3243												25 Ne 27					
371 Na 1156	922 Mg 1363												84 Ar 87					
337 K 1047	1112 Ca 1757	1814 3104	1933 3560	1973 3650	2130 2755	1517 2235	1808 3023	1768 3143	1726 3005	1357 2840	693 1180	303 2676	1211 3103	490 886	266 958	117 332	Kr 121	
312 Rb 961	1042 Sr 1657	1780 3611	2125 4650	2741 5015	2890 4885	2445 5150	2583 4173	2239 4000	1825 3413	1235 2485	594 1038	429 2353	505 2543	904 2023	723 1263	387 458	161 166	Xe 166
302 Cs 952	983 Ba 2023	1194 3730	2503 5470	3269 5698	3680 5930	3453 5900	3327 5300	2683 4403	2045 4100	1338 3080	234 630	577 1730	601 2013	545 1833	527 1235	575 610	202 211	Rn
300 Fr 950	973 Ra 1413	1320 3470																

9. Covalent bond lengths

Bond	Bond length (nm)	Bond	Bond length (nm)
H–H	0.074	C–H	0.109
C–C	0.154	Si–H	0.146
C=C	0.134	N–H	0.101
C≡C	0.120	P–H	0.142
C–C (in benzene)	0.139	O–H	0.096
Si–Si	0.235	S–H	0.135
N–N	0.146	F–H	0.092
N=N	0.120	Cl–H	0.128
N≡N	0.110	Br–H	0.141
P–P (P_4)	0.221	I–H	0.160
O–O	0.148	C–O	0.143
O=O	0.121	C=O	0.122
S–S (S_8)	0.207	C–O (in phenol)	0.136
S=S	0.188	C–N	0.147
F–F	0.142	C=N	0.127
Cl–Cl	0.199	C≡N	0.116
Br–Br	0.228	C–N (in phenylamine)	0.135
I–I	0.267	C–F	0.138
		C–Cl	0.177
		C–Cl (in chlorobenzene)	0.169
		C–Br	0.193
		C–I	0.214
		Si–O	0.150

10. Average bond enthalpies at 298 K

Bond	$\Delta H \text{ (kJ mol}^{-1}\text{)}$	Bond	$\Delta H \text{ (kJ mol}^{-1}\text{)}$
H–H	436	C–H	412
D–D	442	Si–H	318
C–C	348	N–H	388
C=C	612	P–H	322
C≡C	837	O–H	463
C–C (benzene)	518	S–H	338
Si–Si	226	F–H	562
Ge–Ge	188	Cl–H	431
Sn–Sn	151	Br–H	366
N–N	163	I–H	299
N=N	409	C–O	360
N≡N	944	C=O	743
P–P	172	C–N	305
O–O	146	C=N	613
O=O	496	C≡N	890
S–S	264	C–F	484
F–F	158	C–Cl	338
Cl–Cl	242	C–Br	276
Br–Br	193	C–I	238
I–I	151	Si–O	374

III. Organic compounds—thermodynamic data

Substance	Formula	State	ΔH_f^\ominus (kJ mol ⁻¹)	ΔG_f^\ominus (kJ mol ⁻¹)	S^\ominus (J K ⁻¹ mol ⁻¹)
methane	CH ₄	g	-75	-51	186
ethane	C ₂ H ₆	g	-85	-33	230
propane	C ₃ H ₈	g	-104	-24	270
butane	C ₄ H ₁₀	g	-125	-16	310
pentane	C ₅ H ₁₂	l	-173	-9	261
hexane	C ₆ H ₁₄	l	-199	-4	296
ethene	C ₂ H ₄	g	52	68	219
propene	C ₃ H ₆	g	20	63	267
but-1-ene	C ₄ H ₈	g	1	72	307
<i>cis</i> -but-2-ene	C ₄ H ₈	g	-6	67	301
<i>trans</i> -but-2-ene	C ₄ H ₈	g	-10	64	296
ethyne	C ₂ H ₂	g	227	209	201
propyne	C ₃ H ₄	g	185	194	248
buta-1,3-diene	C ₄ H ₆	g	112	152	279
cyclohexane	C ₆ H ₁₂	l	-156	27	204
benzene	C ₆ H ₆	g	83	130	269
benzene	C ₆ H ₆	l	49	125	173
methylbenzene	C ₆ H ₅ CH ₃	l	12	111	320
ethylbenzene	C ₆ H ₅ CH ₂ CH ₃	l	13	120	255
phenylethene	C ₆ H ₅ CHCH ₂	l	104	202	345
chloromethane	CH ₃ Cl	g	-82	-59	234
dichloromethane	CH ₂ Cl ₂	l	-117	-63	179
trichloromethane	CHCl ₃	l	-132	-72	203
bromomethane	CH ₃ Br	g	-36	-26	246
tribromomethane	CHBr ₃	l	-20	3	222
iodomethane	CH ₃ I	l	-8	20	163
triodomethane	CHI ₃	s	141		
chloroethane	C ₂ H ₅ Cl	g	-105	-53	276
bromoethane	C ₂ H ₅ Br	l	-85		

Substance	Formula	State	ΔH_f^\ominus (kJ mol ⁻¹)	ΔG_f^\ominus (kJ mol ⁻¹)	S^\ominus (J K ⁻¹ mol ⁻¹)
iodoethane	C ₂ H ₅ I	l	-31		
chloroethene	C ₂ H ₃ Cl	g	31	52	264
1,2-dichloroethane	CH ₂ ClCH ₂ Cl	l	-166	-80	208
chlorobenzene	C ₆ H ₅ Cl	l	11	94	314
methanol	CH ₃ OH	g	-201	-162	238
methanol	CH ₃ OH	l	-239	-166	127
ethanol	C ₂ H ₅ OH	g	-235	-169	282
ethanol	C ₂ H ₅ OH	l	-278	-175	161
phenol	C ₆ H ₅ OH	s	-163	-51	146
methanal	HCHO	g	-116	-110	219
ethanal	CH ₃ CHO	g	-166	-134	266
propanone	(CH ₃) ₂ CO	l	-216	-152	295
methanoic acid	HCOOH	l	-409	-346	129
ethanoic acid	CH ₃ COOH	l	-487	-392	160
benzoic acid	C ₆ H ₅ COOH	s	-385	-245	167
ethyl ethanoate	CH ₃ COOC ₂ H ₅	l	-481		
ethanamide	CH ₃ CONH ₂	s	-320		
methylamine	CH ₃ NH ₂	g	-28	28	242
ethylamine	C ₂ H ₅ NH ₂	g	-49	37	285
urea	CO(NH ₂) ₂	s	-333	-47	105

12. Enthalpies of combustion

The values of the molar enthalpy of combustion (ΔH_c^\ominus) in the following table refer to a temperature of 298 K and a pressure of 1.01×10^5 Pa (1 atm).

Substance	Formula	State	ΔH_c^\ominus (kJ mol ⁻¹)	Substance	Formula	State	ΔH_c^\ominus (kJ mol ⁻¹)
hydrogen	H ₂	g	-286	propan-1-ol	C ₃ H ₇ OH	l	-2010
sulfur	S	s	-297	butan-1-ol	C ₄ H ₉ OH	l	-2673
carbon (graphite)	C	s	-394	phenylmethanol	C ₆ H ₅ CH ₂ OH	l	-4056
carbon (diamond)	C	s	-395	cyclohexanol	C ₆ H ₁₁ OH	s	-3727
carbon monoxide	CO	g	-283	phenol	C ₆ H ₅ OH	s	-3064
methane	CH ₄	g	-890	ethoxyethane	(C ₂ H ₅) ₂ O	l	-2727
ethane	C ₂ H ₆	g	-1560	methanal	HCHO	g	-561
propane	C ₃ H ₈	g	-2220	ethanal	CH ₃ CHO	l	-1167
butane	C ₄ H ₁₀	g	-2877	benzaldehyde	C ₆ H ₅ CHO	l	-3520
pentane	C ₅ H ₁₂	g	-3509	propanone	(CH ₃) ₂ CO	l	-1786
hexane	C ₆ H ₁₄	l	-4194	pentan-3-one	(C ₂ H ₅) ₂ CO	l	-3078
octane	C ₈ H ₁₈	l	-5512	phenylethanone	CH ₃ COC ₆ H ₅	s	-4138
cyclohexane	C ₆ H ₁₂	l	-3924	diphenylmethanone	(C ₆ H ₅) ₂ CO	s	-6512
ethene	C ₂ H ₄	l	-1409	methanoic acid	HCOOH	l	-263
buta-1,3-diene	C ₄ H ₆	g	-2542	ethanoic acid	CH ₃ COOH	l	-876
ethyne	C ₂ H ₂	g	-1299	benzoic acid	C ₆ H ₅ COOH	s	-3227
benzene	C ₆ H ₆	l	-3267	ethanedioic acid	(COOH) ₂	s	-246
methylbenzene	C ₆ H ₅ CH ₃	l	-3909	ethyl ethanoate	CH ₃ COOC ₂ H ₅	l	-2246

Substance	Formula	State	ΔH_c^\ominus (kJ mol $^{-1}$)	Substance	Formula	State	ΔH_c^\ominus (kJ mol $^{-1}$)
naphthalene	C ₁₀ H ₈	l	-5157	ethanamide	CH ₃ CONH ₂	s	-1182
anthracene	C ₁₄ H ₁₀	s	-7114	benzamide	C ₆ H ₅ CONH ₂	s	-3546
chloroethane	C ₂ H ₅ Cl	g	-1413	methylamine	CH ₃ NH ₂	g	-1072
bromoethane	C ₂ H ₅ Br	l	-1425	ethylamine	C ₂ H ₅ NH ₂	g	-1709
iodoethane	C ₂ H ₅ I	l	-1466	phenylamine	C ₆ H ₅ NH ₂	l	-3397
(chloromethyl)benzene	C ₆ H ₅ CH ₂ Cl	l	-3709	nitrobenzene	C ₆ H ₅ NO ₂	l	-3094
trichloromethane	CHCl ₃	l	-373	urea	CO(NH ₂) ₂	s	-634
methanol	CH ₃ OH	l	-715	glucose	C ₆ H ₁₂ O ₆	s	-2816
ethanol	C ₂ H ₅ OH	l	-1371	sucrose	C ₁₂ H ₂₂ O ₁₁	s	-5644

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
 $\text{MX(s)} \rightarrow \text{M}^{+}(\text{g}) + \text{X}^{-}(\text{g})$
in which the gaseous ions of a crystal are separated to an infinite distance from each other.

Experimental values

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

Alkali metal halides	$\Delta H_{\text{lattice}}^{\ominus}$ (kJ mol ⁻¹)			
	F	Cl	Br	I
Li	1022	846	800	744
Na	902	771	733	684
K	801	701	670	629
Rb	767	675	647	609
Cs	716	645	619	585
Other substances	$\Delta H_{\text{lattice}}^{\ominus}$ (kJ mol ⁻¹)	Other substances	$\Delta H_{\text{lattice}}^{\ominus}$ (kJ mol ⁻¹)	
CaF ₂	2602	MgS	3238	
BeCl ₂	3006	CaS	2966	
MgCl ₂	2493	SrS	2779	
CaCl ₂	2237	BaS	2643	
SrCl ₂	2112	CuCl	976	
BaCl ₂	2018	AgF	955	
MgO	3889	AgCl	905	
CaO	3513	AgBr	890	
SrO	3310	AgI	876	
BaO	3152	NH ₄ Cl	640	

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	$\Delta H_{\text{lattice}}^{\ominus}$ (kJ mol ⁻¹)			
	F	Cl	Br	I
Li	1004	833	787	728
Na	891	766	732	686
K	795	690	665	632
Rb	761	674	644	607
Cs	728	636	611	582

Other substances	$\Delta H_{\text{lattice}}^{\ominus}$ (kJ mol ⁻¹)	Other substances	$\Delta H_{\text{lattice}}^{\ominus}$ (kJ mol ⁻¹)
CaF ₂	2611	AgF	870
MgO	3929	AgCl	770
CaO	3477	AgBr	758
SrO	3205	AgI	736
BaO	3042		

I4. Standard electrode potentials

Oxidized species	\rightleftharpoons	Reduced species	E^\ominus (V)
$\text{Li}^+(\text{aq}) + \text{e}^-$	\rightleftharpoons	Li(s)	-3.03
$\text{K}^+(\text{aq}) + \text{e}^-$	\rightleftharpoons	K(s)	-2.92
$\text{Ca}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	Ca(s)	-2.87
$\text{Na}^+(\text{aq}) + \text{e}^-$	\rightleftharpoons	Na(s)	-2.71
$\text{Mg}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	Mg(s)	-2.36
$\text{Al}^{3+}(\text{aq}) + 3\text{e}^-$	\rightleftharpoons	Al(s)	-1.66
$\text{Mn}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	Mn(s)	-1.18
$\text{H}_2\text{O(l)} + \text{e}^-$	\rightleftharpoons	$\frac{1}{2}\text{H}_2(\text{g}) + \text{OH}^-(\text{aq})$	-0.83
$\text{Zn}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	Zn(s)	-0.76
$\text{Fe}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	Fe(s)	-0.44
$\text{Ni}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	Ni(s)	-0.23
$\text{Sn}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	Sn(s)	-0.14
$\text{Pb}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	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	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	Cu(s)	+0.52

Oxidized species	\rightleftharpoons	Reduced species	E^\ominus (V)
$\frac{1}{2}\text{I}_2(\text{s}) + \text{e}^-$	\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	$\text{Br}^-(\text{aq})$	+1.09
$\frac{1}{2}\text{O}_2(\text{g}) + 2\text{H}^+(\text{aq}) + 2\text{e}^-$	\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 ₃ COOH	4.76
propanoic	CH ₃ CH ₂ COOH	4.87
butanoic	CH ₃ (CH ₂) ₂ COOH	4.82
2-methylpropanoic	(CH ₃) ₂ CHCOOH	4.85
pentanoic	CH ₃ (CH ₂) ₃ COOH	4.86
2,2-dimethylpropanoic	(CH ₃) ₃ CCOOH	5.05
benzoic	C ₆ H ₅ COOH	4.20
phenylethanoic	C ₆ H ₅ CH ₂ COOH	4.31

Halogenated carboxylic acids

Name	Formula	pK_a
chloroethanoic	CH ₂ ClCOOH	2.86
dichloroethanoic	CHCl ₂ COOH	1.29
trichloroethanoic	CCl ₃ COOH	0.65
fluoroethanoic	CH ₂ FCOOH	2.66
bromoethanoic	CH ₂ BrCOOH	2.90
iodoethanoic	CH ₂ I ⁻ COO ⁻	3.17

Phenols

Name	Formula	pK_a
phenol	C_6H_5OH	10.00
2-nitrophenol	$O_2NC_6H_4OH$	7.21
3-nitrophenol	$O_2NC_6H_4OH$	8.35
4-nitrophenol	$O_2NC_6H_4OH$	7.15
2,4-dinitrophenol	$(O_2N)_2C_6H_3OH$	4.01
2,4,6-trinitrophenol	$(O_2N)_3C_6H_2OH$	0.42

Alcohols

Name	Formula	pK_a
methanol	CH_3OH	15.5
ethanol	C_2H_5OH	16.0

Amines

Name	Formula	pK_b
ammonia	NH_3	4.75
methylamine	CH_3NH_2	3.36
ethylamine	$CH_3CH_2NH_2$	3.27
dimethylamine	$(CH_3)_2NH$	3.28
trimethylamine	$(CH_3)_3N$	4.20
diethylamine	$(C_2H_5)_2NH$	3.07
triethylamine	$(C_2H_5)_3N$	3.36
phenylamine	$C_6H_5NH_2$	9.38

16. Acid–base indicators

Indicator	pK_a	pH range	Colour change	
			Acid	Alkali
methyl orange	3.7	3.1–4.4	red	yellow
bromophenol blue	4.0	3.0–4.6	yellow	blue
bromocresol green	4.7	3.8–5.4	yellow	blue
methyl red	5.1	4.2–6.3	red	yellow
bromothymol blue	7.0	6.0–7.6	yellow	blue
phenol red	7.9	6.8–8.4	yellow	red
phenolphthalein	9.3	8.3–10.0	colourless	red

17. Infrared data

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

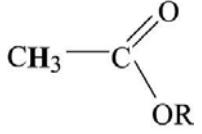
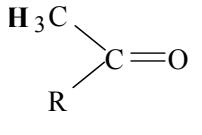
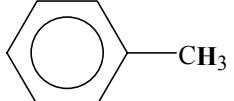
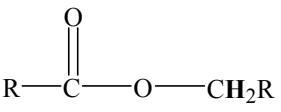
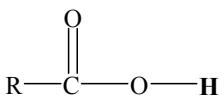
Bond	Organic molecules	Wavenumber (cm^{-1})
C—I	iodoalkanes	490–620
C—Br	bromoalkanes	500–600
C—Cl	chloroalkanes	600–800
C—F	fluoroalkanes	1000–1400
C—O	alcohols, esters, ethers	1050–1410
C=C	alkenes	1610–1680
C=O	aldehydes, ketones, acids, esters	1700–1750
C≡C	alkynes	2100–2260
O—H	“hydrogen bonded”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

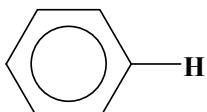
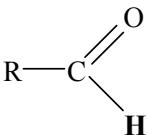
18. ^1H NMR data

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)
$\text{R}-\text{CH}_3$	0.9–1.0
$\text{R}-\text{CH}_2-\text{R}$	1.3–1.4
R_3CH	1.4–1.6
	2.0–2.5
	2.2–2.7
	2.5–3.5
$\text{R}-\text{C}\equiv\text{C}-\text{H}$	1.8–3.1
$\text{R}-\text{CH}_2-\text{Hal}$	3.5–4.4
$\text{R}-\text{O}-\text{CH}_3$	3.3–3.7
	3.8–4.1
	9.0–13.0
$\text{R}-\text{O}-\text{H}$	4.0–12.0

Type of proton	Chemical shift (ppm)
RHC=CH ₂	4.5–6.0
	4.0–12.0
	6.9–9.0
	9.4–10.0

19. 2-Amino acids

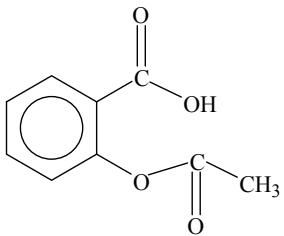
Common name	Symbol	Structural formula	pH of isoelectric point
alanine	Ala	$\text{H}_2\text{N}-\underset{\text{CH}_3}{\text{CH}}-\text{COOH}$	6.0
arginine	Arg	$\text{H}_2\text{N}-\underset{\text{CH}_2-\text{CH}_2-\text{CH}_2}{\text{CH}}-\text{NH}-\underset{\text{NH}}{\overset{\parallel}{\text{C}}}-\text{NH}_2$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

Common name	Symbol	Structural formula	pH of isoelectric point
histidine	His	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{C}=\text{N}-\text{H} \\ \\ \text{N}=\text{C} \end{array}$	7.6
isoleucine	Ile	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_3-\text{CH}-\text{CH}_2-\text{CH}_3 \end{array}$	6.0
leucine	Leu	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2 \\ \\ \text{CH}_3-\text{CH}-\text{CH}_3 \end{array}$	6.0
lysine	Lys	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{NH}_2 \end{array}$	9.7
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	$\begin{array}{c} \text{H} \\ \\ \text{N} \\ \\ \text{COOH} \\ \text{C} \\ \\ \text{C} \end{array}$	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	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_3-\text{CH}-\text{OH} \end{array}$	5.6

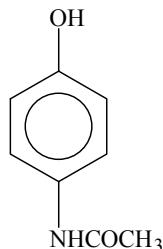
2-Amino acids

Common name	Symbol	Structural formula	pH of isoelectric point
tryptophan	Trp	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{C}=\text{N}-\text{C}_6\text{H}_5 \end{array}$	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	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_3-\text{CH}-\text{CH}_3 \end{array}$	6.0

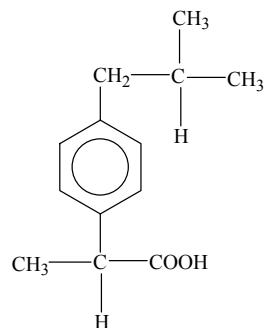
20. Structural formulas of some important medicines and drugs



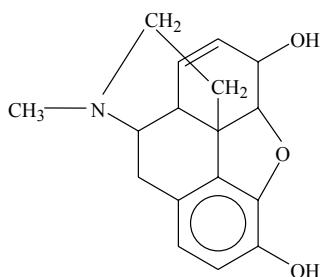
aspirin



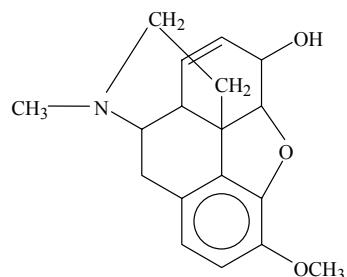
paracetamol
(acetaminophen)



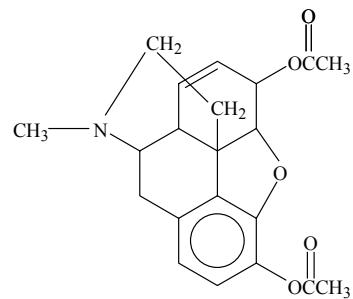
ibuprofen



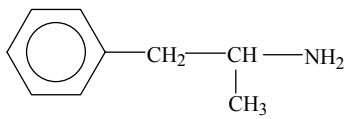
morphine



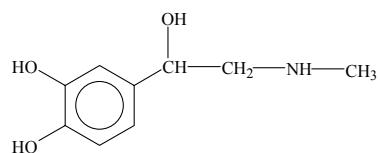
codeine



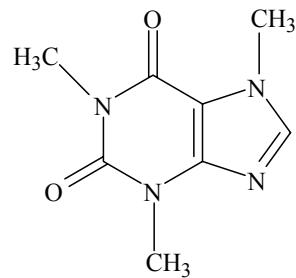
heroin



amphetamine

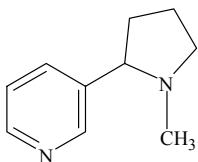


epinephrine (adrenaline)

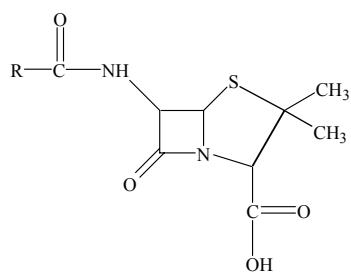


caffeine

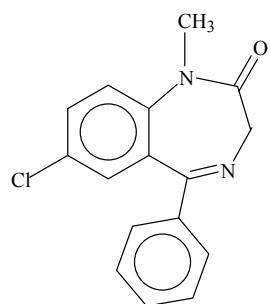
Structural formulas of some important medicines and drugs



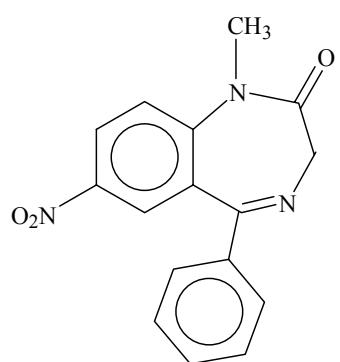
nicotine



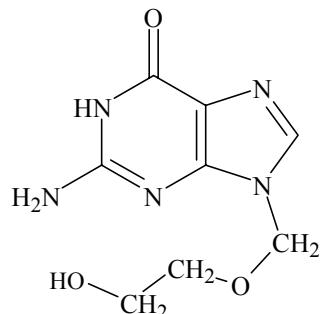
penicillin



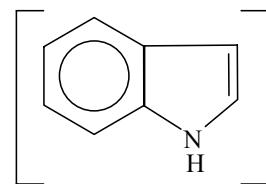
diazepam (Valium[®])



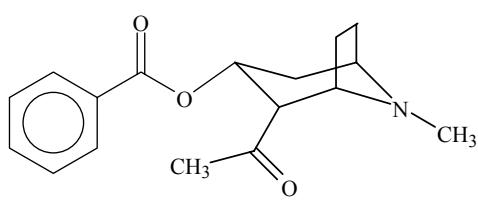
nitrazepam (Mogadon[®])



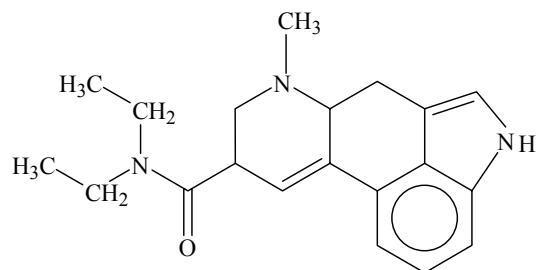
acyclovir



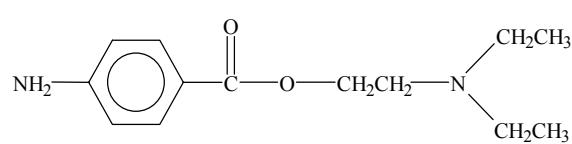
indole



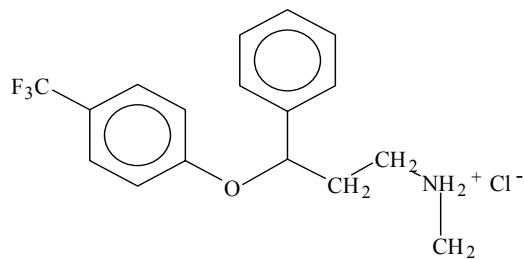
cocaine



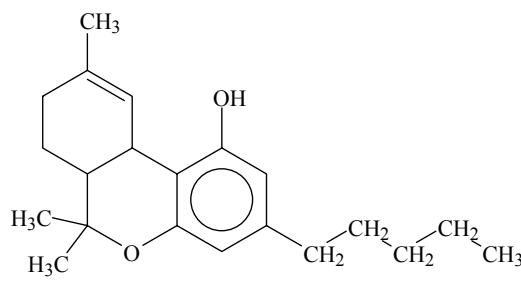
lysergic acid diethylamide (LSD)



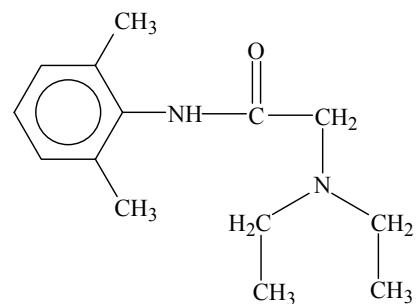
procaine



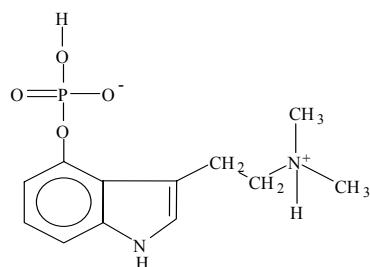
fluoxetine hydrochloride (Prozac[®])



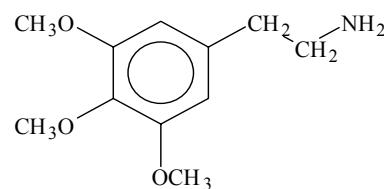
tetrahydrocannabinol (THC)



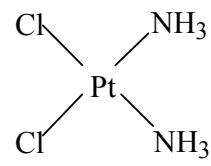
lidocaine



psilocybine

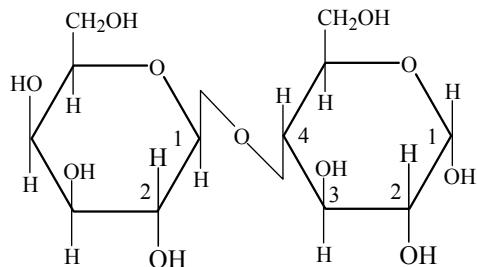


mescaline

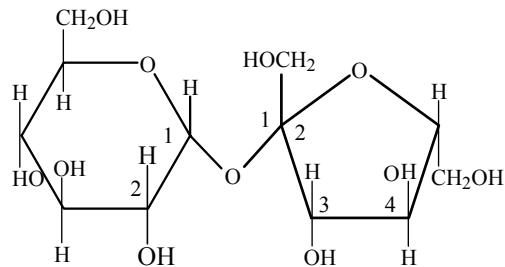


cisplatin

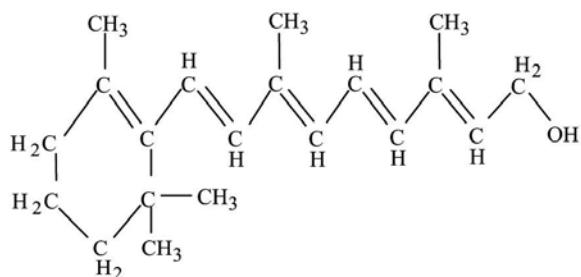
21. Structural formulas of some important biological molecules



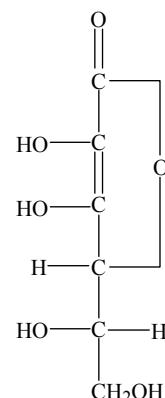
lactose



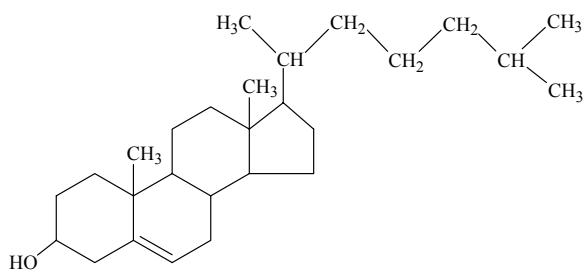
sucrose



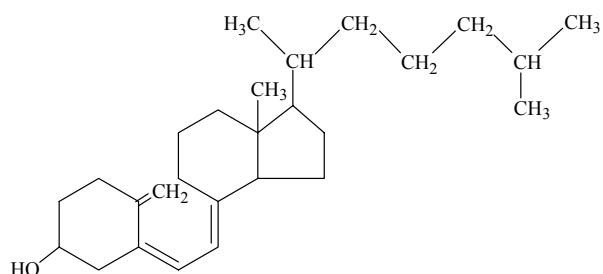
retinol (vitamin A)



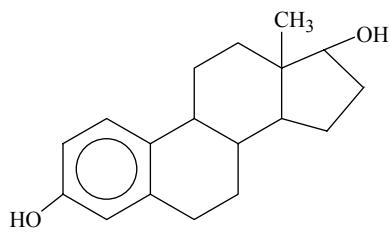
ascorbic acid (vitamin C)



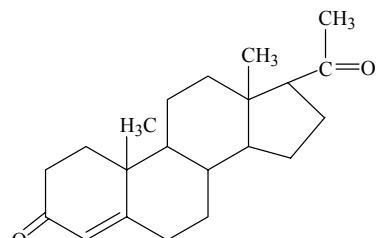
cholesterol



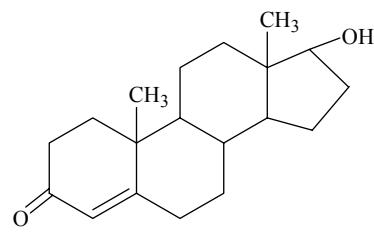
vitamin D



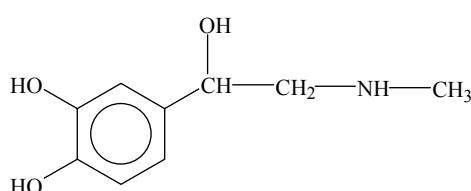
estradiol



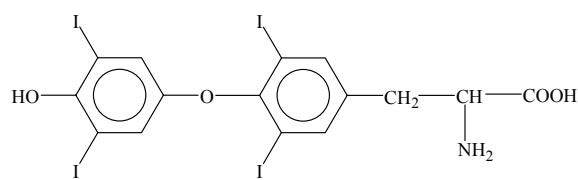
progesterone



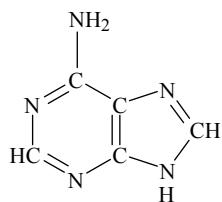
testosterone



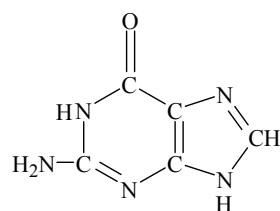
epinephrine (adrenaline)



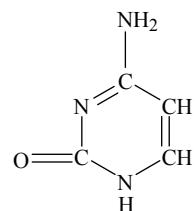
thyroxine



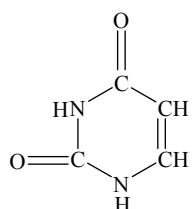
adenine



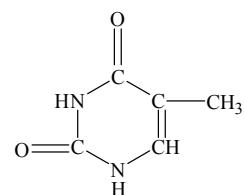
guanine



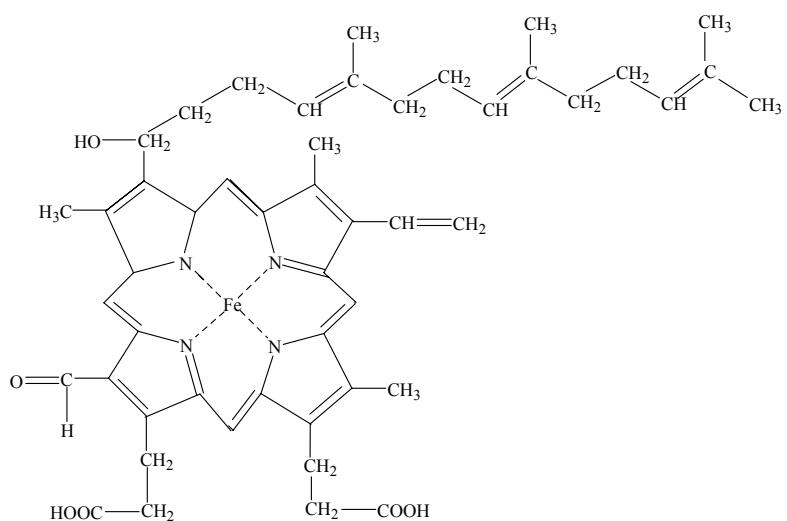
cytosine



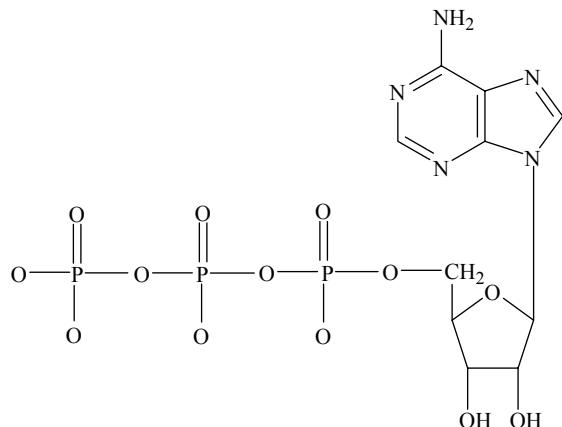
uracil



thymine



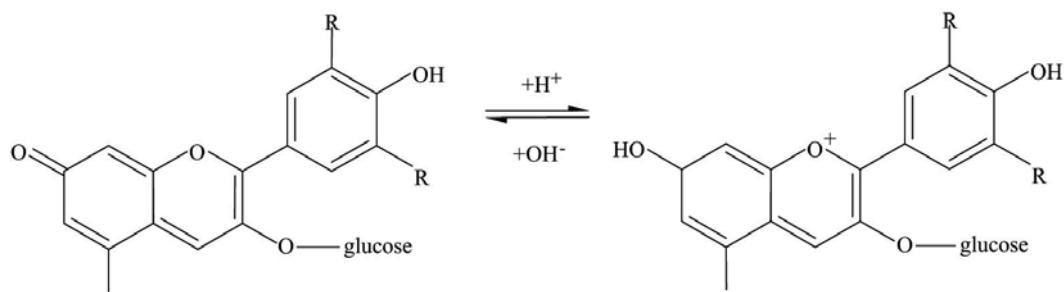
the heme group from cytochrome oxidase



adenosine triphosphate (ATP)

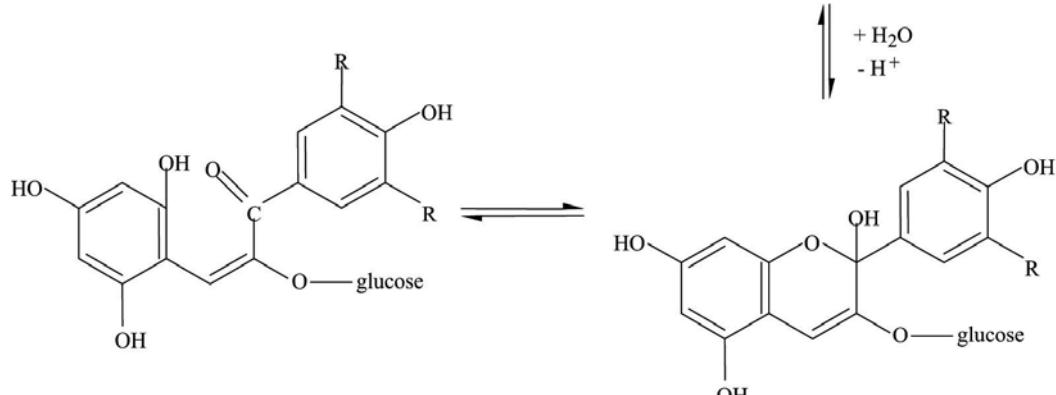
22. Structural formulas of some important food chemistry molecules

Some anthocyanins



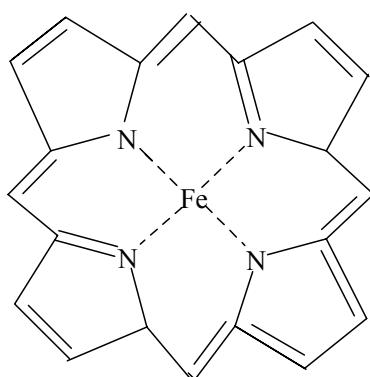
quinoidal base (blue)

flavylium cation (red)

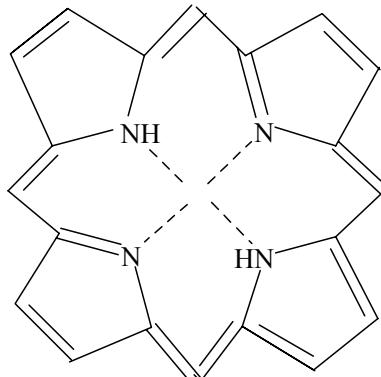


chalcone (colourless)

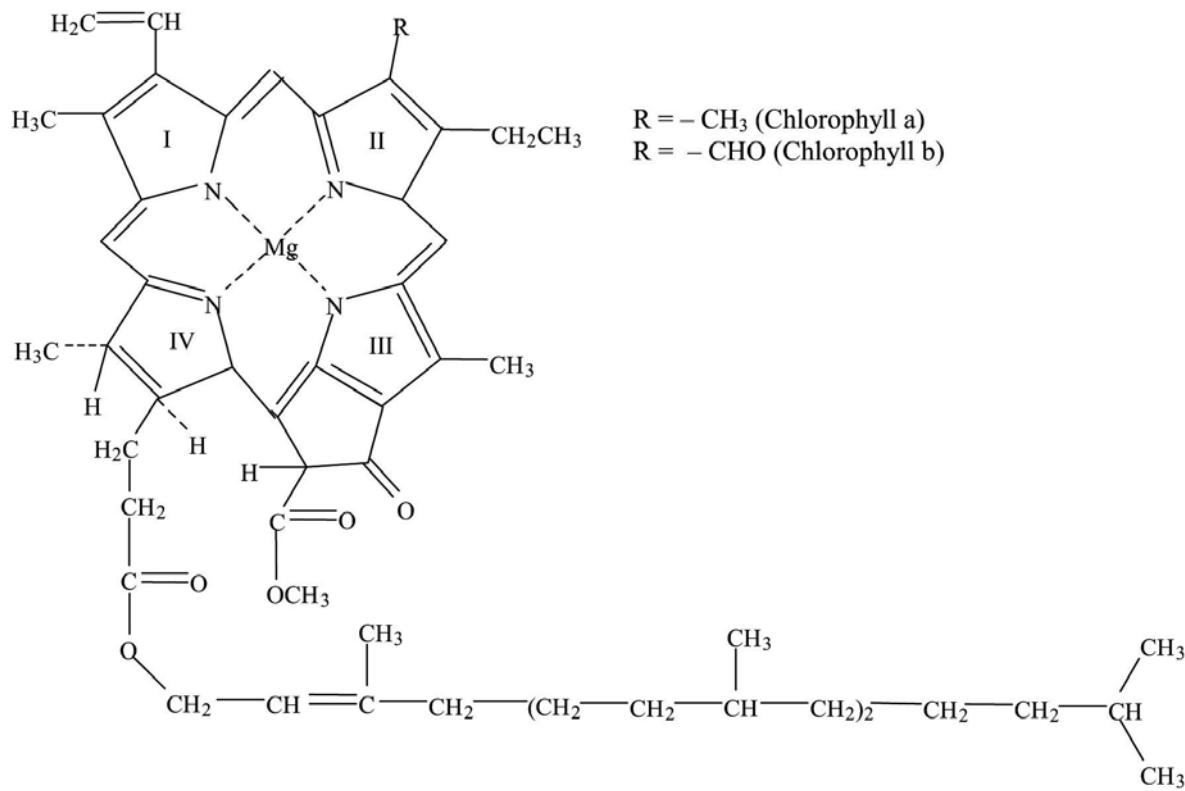
carbinol pseudo-base (colourless)



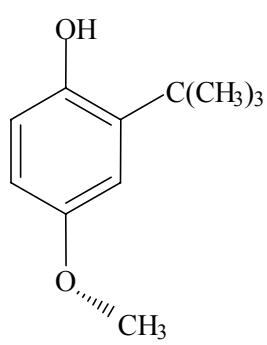
myoglobin



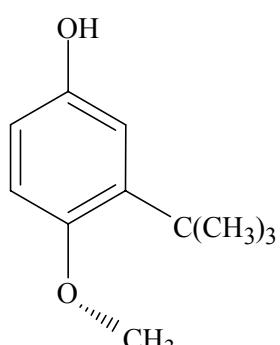
porphyrin



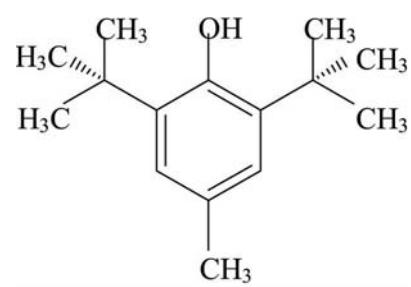
Some preservatives



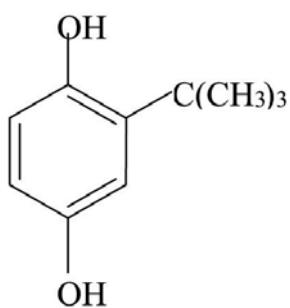
2-*tert*-butyl-4-hydroxyanisole (2-BHA)



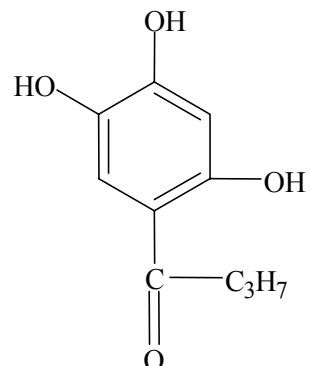
3-*tert*-butyl-4-hydroxyanisole (3-BHA)



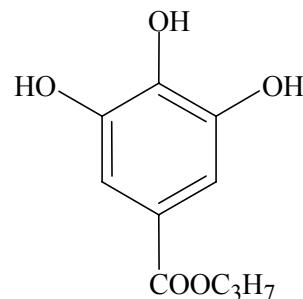
3,5-di-*tert*-butyl-4-hydroxytoluene (BHT)



tert-butylhydroquinone (TBHQ)

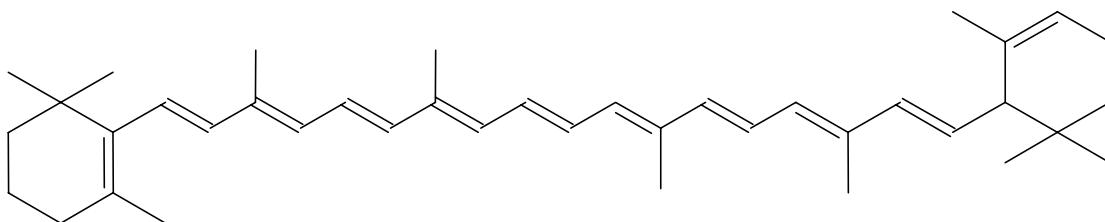


2,4,5-trihydroxybutyrophenone (THBP)

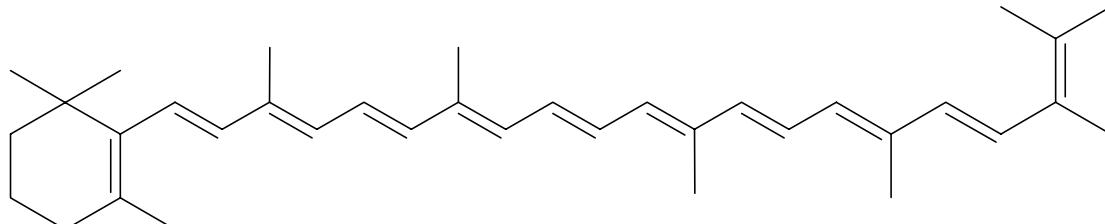


propyl gallate (PG)

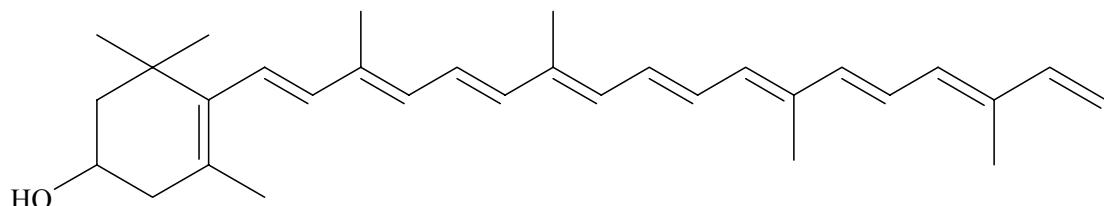
Some of the carotenes



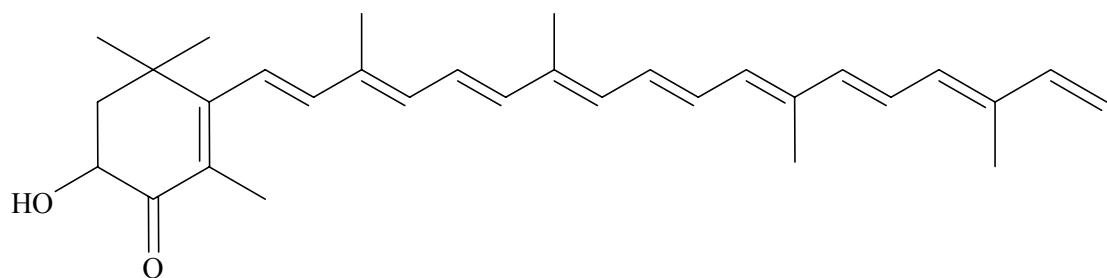
alpha-carotene



beta-carotene



lutein



astaxanthin

Some 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	$\text{CH}_3(\text{CH}_2)_{14}\text{COOH}$
Palmitic acid	$\text{CH}_3(\text{CH}_2)_{14}\text{COOH}$
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	$\text{CH}_3\text{CH}_2(\text{CH}=\text{CHCH}_2)_3(\text{CH}_2)_6\text{COOH}$

