

Chemistry data booklet

First assessment 2016

Fourth edition



International Baccalaureate®
Baccalauréat International
Bachillerato Internacional

Diploma Programme

Chemistry data booklet

Published June 2014
Updated January 2016
Updated January 2017

Published on behalf of the International Baccalaureate Organization, a not-for-profit educational foundation of 15 Route des Morillons, 1218 Le Grand-Saconnex, Geneva, Switzerland by the

International Baccalaureate Organization (UK) Ltd
Peterson House, Malthouse Avenue, Cardiff Gate
Cardiff, Wales CF23 8GL
United Kingdom
Website: www.ibo.org

© International Baccalaureate Organization 2014

The International Baccalaureate Organization (known as the IB) offers four high-quality and challenging educational programmes for a worldwide community of schools, aiming to create a better, more peaceful world. This publication is one of a range of materials produced to support these programmes.

The IB may use a variety of sources in its work and checks information to verify accuracy and authenticity, particularly when using community-based knowledge sources such as Wikipedia. The IB respects the principles of intellectual property and makes strenuous efforts to identify and obtain permission before publication from rights holders of all copyright material used. The IB is grateful for permissions received for material used in this publication and will be pleased to correct any errors or omissions at the earliest opportunity.

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, without the prior written permission of the IB, or as expressly permitted by law or by the IB's own rules and policy. See <http://www.ibo.org/copyright>.

IB merchandise and publications can be purchased through the IB store at <http://store.ibo.org>.

Email: sales@ibo.org

Contents

1. Some relevant equations	1
2. Physical constants and unit conversions	2
3. The electromagnetic spectrum	3
4. Fundamental particles	3
5. Names of the elements	4
6. The periodic table	6
7. Melting points and boiling points of the elements (at 101.325 kPa)	7
8. First ionization energy, electron affinity and electronegativity of the elements	8
9. Atomic and ionic radii of the elements	9
10. Covalent bond lengths	10
11. Bond enthalpies and average bond enthalpies at 298 K	11
12. Selected compounds—thermodynamic data	12
13. Enthalpies of combustion	13
14. Common oxidation states of the 3d ions	14
15. Spectrochemical series	14
16. Ligands	15
17. Colour wheel	15
18. Lattice enthalpies at 298 K (experimental values)	16
19. Enthalpies of aqueous solutions	17
20. Enthalpies of hydration	18
21. Strengths of organic acids and bases	19
22. Acid-base indicators	21
23. Values of the ionization constant of water	22
24. Standard electrode potentials at 298 K	23
25. Activity series	24
26. Infrared data	25
27. ^1H NMR data	26
28. Mass spectral fragments lost	27
29. Triangular bonding diagram	28
30. Resin identification codes	29
31. Representations of some materials molecules	29

32. Solubility product constants at 298 K	30
33. 2-amino acids	31
34. Lipids, carbohydrates and nucleotide components	33
35. Vitamins and pigments	35
36. Binding energy curve	37
37. Representations of some medicinal molecules.	38
38. References	40

Notes

This booklet cannot be used for paper 1 of the examination (SLP1 and HLP1), but the periodic table given in section 6 will be available as part of these examination papers. Clean copies of this booklet must be made available to candidates for papers 2 and 3 (SLP2, HLP2, SLP3 and HLP3).

1. Some relevant equations

Topic	Equation
1.3	$pV = nRT$
2.2 and C.4	$c = v\lambda$
5.1	$q = mc\Delta T$
8.3	$pH = -\log_{10} [H_3O^+]$ or $pH = -\log_{10} [H^+]$
12.1	$E = h\nu$
15.2	$\Delta G^\ominus = \Delta H^\ominus - T\Delta S^\ominus$
16.2	$k = Ae^{\frac{-E_a}{RT}}$
16.2	$\ln k = \frac{-E_a}{RT} + \ln A$
16.2	$\ln \frac{k_1}{k_2} = \frac{E_a}{R} \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$
17.1	$\Delta G^\ominus = -RT \ln K$
19.1	$\Delta G^\ominus = -nFE^\ominus$
A.5	$\% \text{ atom economy} = \frac{\text{total mass of desired product}}{\text{total mass of all reactants}} \times 100$
A.8	$n\lambda = 2d \sin \theta$
B.7 and D.4	$pH = pK_a + \log \left(\frac{[A^-]}{[HA]} \right)$
B.7	$\log_{10} \frac{I_0}{I} = \epsilon lc$

Topic	Equation
C.1	Energy density = $\frac{\text{energy released from fuel}}{\text{volume of fuel consumed}}$
C.1	Specific energy = $\frac{\text{energy released from fuel}}{\text{mass of fuel consumed}}$
C.3	$N = N_0 e^{-\lambda t}$
C.3 and D.8	$t_{\frac{1}{2}} = \frac{\ln 2}{\lambda}$
C.6	$E = E^\ominus - \left(\frac{RT}{nF} \right) \ln Q$
C.7	$\frac{\text{Rate}_1}{\text{Rate}_2} = \sqrt{\frac{M_2}{M_1}}$
D.8	$N(t) = N_0 \left(\frac{1}{2} \right)^{\frac{t}{t_{1/2}}}$

2. Physical constants and unit conversions

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

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

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

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

STP conditions = 273 K and 100 kPa

SATP conditions = 298 K and 100 kPa

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

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

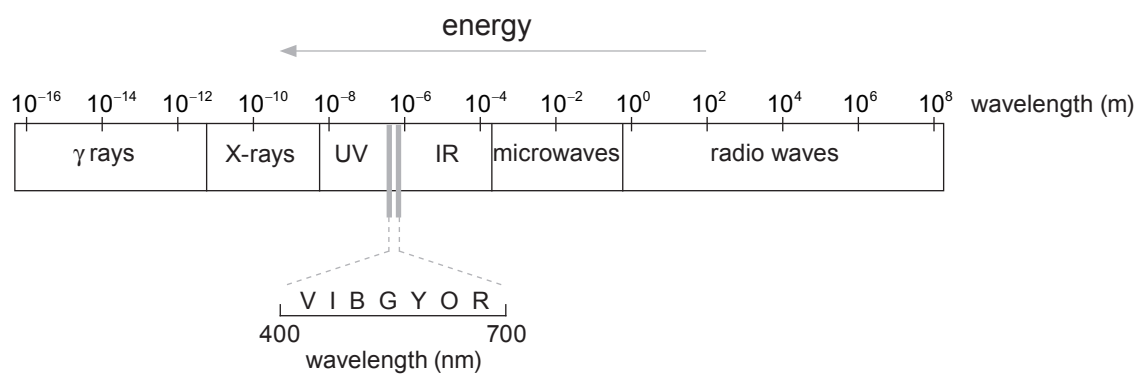
Planck's constant (h) = $6.63 \times 10^{-34} \text{ J s}$

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

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

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

3. The electromagnetic spectrum



4. Fundamental particles

	Proton	Neutron	Electron
Mass (kg)	1.672622×10^{-27}	1.674927×10^{-27}	9.109383×10^{-31}
Charge (C)	1.602189×10^{-19}	0	1.602189×10^{-19}

5. Names of the elements

Element	Symbol	Atomic number
actinium	Ac	89
aluminium	Al	13
americium	Am	95
antimony	Sb	51
argon	Ar	18
arsenic	As	33
astatine	At	85
barium	Ba	56
berkelium	Bk	97
beryllium	Be	4
bismuth	Bi	83
bohrium	Bh	107
boron	B	5
bromine	Br	35
cadmium	Cd	48
caesium	Cs	55
calcium	Ca	20
californium	Cf	98
carbon	C	6
cerium	Ce	58
chlorine	Cl	17
chromium	Cr	24
cobalt	Co	27
copernicium	Cn	112
copper	Cu	29
curium	Cm	96
darmstadtium	Ds	110
dubnium	Db	105

Element	Symbol	Atomic number
dysprosium	Dy	66
einsteinium	Es	99
erbium	Er	68
europium	Eu	63
fermium	Fm	100
fluorine	F	9
francium	Fr	87
gadolinium	Gd	64
gallium	Ga	31
germanium	Ge	32
gold	Au	79
hafnium	Hf	72
hassium	Hs	108
helium	He	2
holmium	Ho	67
hydrogen	H	1
indium	In	49
iodine	I	53
iridium	Ir	77
iron	Fe	26
krypton	Kr	36
lanthanum	La	57
lawrencium	Lr	103
lead	Pb	82
lithium	Li	3
lutetium	Lu	71
magnesium	Mg	12
manganese	Mn	25

Element	Symbol	Atomic number
meitnerium	Mt	109
mendelevium	Md	101
mercury	Hg	80
molybdenum	Mo	42
neodymium	Nd	60
neon	Ne	10
neptunium	Np	93
nickel	Ni	28
niobium	Nb	41
nitrogen	N	7
nobelium	No	102
osmium	Os	76
oxygen	O	8
palladium	Pd	46
phosphorus	P	15
platinum	Pt	78
plutonium	Pu	94
polonium	Po	84
potassium	K	19
praseodymium	Pr	59
promethium	Pm	61
protactinium	Pa	91
radium	Ra	88
radon	Rn	86
rhenium	Re	75
rhodium	Rh	45
roentgenium	Rg	111
rubidium	Rb	37

Element	Symbol	Atomic number
ruthenium	Ru	44
rutherfordium	Rf	104
samarium	Sm	62
scandium	Sc	21
seaborgium	Sg	106
selenium	Se	34
silicon	Si	14
silver	Ag	47
sodium	Na	11
strontium	Sr	38
sulfur	S	16
tantalum	Ta	73
technetium	Tc	43
tellurium	Te	52
terbium	Tb	65
thallium	Tl	81
thorium	Th	90
thulium	Tm	69
tin	Sn	50
titanium	Ti	22
tungsten	W	74
uranium	U	92
vanadium	V	23
xenon	Xe	54
ytterbium	Yb	70
yttrium	Y	39
zinc	Zn	30
zirconium	Zr	40

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18		
1	1 H 1.01																		2 He 4.00	
2	3 Li 6.94	4 Be 9.01																	9 F 19.00	10 Ne 20.18
	11 Na 22.99	12 Mg 24.31																	17 Cl 35.45	18 Ar 39.95
3																				
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.87	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.38	31 Ga 69.72	32 Ge 72.63	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.90		
	37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.96	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 131.29		
5	55 Cs 132.91	56 Ba 137.33	57† La 138.91	72 Hf 178.49	73 Ta 180.95	74 W 183.84	75 Re 186.21	76 Os 190.23	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.20	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)		
	87 Fr (223)	88 Ra (226)	89‡ Ac (227)	104 Rf (267)	105 Db (268)	106 Sg (269)	107 Bh (270)	108 Hs (269)	109 Mt (278)	110 Ds (281)	111 Rg (281)	112 Cn (285)	113 Uut (286)	114 Uuq (289)	115 Uup (288)	116 Uuh (293)	117 Uus (294)	118 Uuo (294)		
7																				
†	58 Ce 140.12	59 Pr 140.91	†	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.05	71 Lu 174.97					
	90 Th 232.04	91 Pa 231.04	‡	92 U 238.03	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)					

Chemistry data booklet

9. Atomic and ionic radii of the elements

32 H	Atomic radius (10 ⁻¹² m)																37 He	
	Element																	
130 Li 76 (1+)	99 Be 45 (2+)	Ionic radius (10 ⁻¹² m)															62 Ne	
	160 Na 102 (1+)	140 Mg 72 (2+)	159 Sc 75 (3+)	148 Ti 86 (2+) 61 (4+)	144 V 79 (2+) 54 (5+)	130 Cr 62 (3+) 44 (6+)	129 Mn 83 (2+) 53 (4+)	124 Fe 61 (2+) 55 (3+)	118 Co 65 (2+) 55 (3+)	117 Ni 69 (2+)	122 Cu 77 (1+) 73 (2+)	120 Zn 74 (2+)	123 Ga 62 (3+)	142 In 80 (3+)	140 Sn 118 (2+) 69 (4+)	136 Sb 76 (3+)		137 Te 221 (2-) 220 (1-)
200 K 138 (1+)	174 Ca 100 (2+)	176 Y 90 (3+)		164 Zr 72 (4+)	156 Nb 72 (3+) 64 (5+)	146 Mo 65 (4+)	138 Tc 65 (4+)	136 Ru 68 (3+) 62 (4+)	134 Rh 67 (3+) 60 (4+)	130 Pd 86 (2+) 62 (4+)	136 Ag 115 (1+)	140 Cd 95 (2+)	142 In 80 (3+)	140 Sn 118 (2+) 69 (4+)	136 I 220 (1-)	136 Xe	136 At	146 Rn
215 Rb 152 (1+)	190 Sr 118 (2+)	194 La 103 (3+)		164 Hf 71 (4+)	158 Ta 64 (5+)	150 W 66 (4+) 60 (6+)	141 Re 63 (4+) 53 (7+)	136 Os 63 (4+) 55 (6+)	132 Ir 68 (3+) 63 (4+)	130 Pt 80 (2+) 63 (4+)	137 (1+) 85 (3+)	132 Hg 119 (1+) 102 (2+)	144 Tl 150 (1+) 89 (3+)	145 Pb 119 (2+) 78 (4+)	150 Bi 103 (3+) 76 (5+)	142 Po 97 (4+)		
238 Cs 167 (1+)	206 Ba 135 (2+)	201 Ac																
242 Fr	211 Ra																	

10. Covalent bond lengths

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

	Br	C	Cl	F	H	I	N	O	P	S	Si
Br	228	194	214	176	141	247	214		220	227	216
C	194	154	177	138	108	214	147	143	184	182	185
Cl	214	177	199	163	128	232	197	170	203	199	202
F	176	138	163	142	92	257	136	142	154	158	156
H	141	108	128	92	74	160	101	97	142	134	148
I	247	214	232	257	160	267			247		243
N	214	147	197	136	101		146	136		175	174
O		143	170	142	97		136	148	154	161	163
P	220	184	203	154	142	247		154	221	210	
S	227	182	199	158	134		175	161	210	205	215
Si	216	185	202	156	148	243	174	163		215	232

Multiple bonds (10^{-12} m = pm)

C=C 134

C≡N 116

N≡N 110

C≡C 120

C=O 122

N=O 114

C=C 140
(in benzene)

C=S 156

O=O 121

C=N 130

N=N 125

S=S 189

11. Bond enthalpies and average bond enthalpies at 298 K

Single bonds (kJ mol^{-1})

	Br	C	Cl	F	H	I	N	O	P	S	Si
Br	193	285	219	249	366	178		201	264	218	330
C	285	346	324	492	414	228	286	358	264	289	307
Cl	219	324	242	255	431	211	192	206	322	271	400
F	249	492	255	159	567	280	278	191	490	327	597
H	366	414	431	567	436	298	391	463	322	364	323
I	178	228	211	280	298	151		201	184		234
N		286	192	278	391		158	214			
O	201	358	206	191	463	201	214	144	363		466
P	264	264	322	490	322	184		363	198		
S	218	289	271	327	364					266	293
Si	330	307	400	597	323	234		466		293	226

Multiple bonds (kJ mol^{-1})

C=C 614	C $\equiv$ N 890	N $\equiv$ N 945
C $\equiv$ C 839	C=O 804	N=O 587
C=C 507 (in benzene)	C=S 536	O=O 498
C=N 615	N=N 470	S=S 429

12. Selected compounds—thermodynamic data

Substance	Formula	State	$\Delta H_f^\ominus$ (kJ mol ⁻¹)	$\Delta G_f^\ominus$ (kJ mol ⁻¹)	$S^\ominus$ (J K ⁻¹ mol ⁻¹)
methane	CH ₄	g	-74.0	-50.0	+186
ethane	C ₂ H ₆	g	-84.0	-32.0	+230
propane	C ₃ H ₈	g	-105	-24.0	+270
butane	C ₄ H ₁₀	g	-126	-17.0	+310
pentane	C ₅ H ₁₂	l	-173		
hexane	C ₆ H ₁₄	l	-199		
ethene	C ₂ H ₄	g	+52.0	+68.0	+220
propene	C ₃ H ₆	g	+20.0	+62.0	+267
but-1-ene	C ₄ H ₈	g	+0.10	+71.0	+306
cis-but-2-ene	C ₄ H ₈	g	-7.0	+66.0	+301
trans-but-2-ene	C ₄ H ₈	g	-11.0	+63.0	+297
ethyne	C ₂ H ₂	g	+228	+211	+201
propyne	C ₃ H ₄	g	+185	+194	+248
buta-1,3-diene	C ₄ H ₆	g	+110	+151	+279
cyclohexane	C ₆ H ₁₂	l	-156		
benzene	C ₆ H ₆	l	+49.0	+125	+173
methylbenzene	C ₆ H ₅ CH ₃	l	+12.0		
ethylbenzene	C ₆ H ₅ CH ₂ CH ₃	l	-12.0		
phenylethene	C ₆ H ₅ CHCH ₂	l	+104		
chloromethane	CH ₃ Cl	g	-82.0	-58.0	+235
dichloromethane	CH ₂ Cl ₂	l	-124		+178
trichloromethane	CHCl ₃	l	-134	-74.0	+202
bromomethane	CH ₃ Br	g	-36.0	-26.0	+246
iodomethane	CH ₃ I	l	-14.0		+163
chloroethane	C ₂ H ₅ Cl	g	-137	-53.0	
bromoethane	C ₂ H ₅ Br	l	-90.0	-26.0	+199
chlorobenzene	C ₆ H ₅ Cl	l	+11.0		
methanol	CH ₃ OH	l	-239	-167	+127
ethanol	C ₂ H ₅ OH	l	-278	-175	+161
phenol	C ₆ H ₅ OH	s	-165		+144
methanal	HCHO	g	-109	-102	+219
ethanal	CH ₃ CHO	g	-166	-133	+264
propanone	(CH ₃) ₂ CO	l	-248		+200
methanoic acid	HCOOH	l	-425	-361	+129
ethanoic acid	CH ₃ COOH	l	-484	-390	+160
benzoic acid	C ₆ H ₅ COOH	s	-385		+168
methylamine	CH ₃ NH ₂	g	-23	+32.0	+243
water	H ₂ O	l	-285.8	-237.1	+70.0
steam	H ₂ O	g	-241.8	-228.6	+188.8
carbon monoxide	CO	g	-110.5	-137.2	+197.7
carbon dioxide	CO ₂	g	-393.5	-394.4	+213.8
hydrogen bromide	HBr	g	-36.3	-53.4	+198.7
hydrogen chloride	HCl	g	-92.3	-95.3	+186.9
hydrogen fluoride	HF	g	-273.3	-275.4	+173.8
hydrogen iodide	HI	g	+26.5	+1.7	+206.6

13. 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 1.00×10^5 Pa.

Substance	Formula	State	$\Delta H_c^\ominus$ (kJ mol ⁻¹)
hydrogen	H ₂	g	-286
sulfur	S	s	-297
carbon (graphite)	C	s	-394
carbon monoxide	CO	g	-283
methane	CH ₄	g	-891
ethane	C ₂ H ₆	g	-1561
propane	C ₃ H ₈	g	-2219
butane	C ₄ H ₁₀	g	-2878
pentane	C ₅ H ₁₂	l	-3509
hexane	C ₆ H ₁₄	l	-4163
octane	C ₈ H ₁₈	l	-5470
cyclohexane	C ₆ H ₁₂	l	-3920
ethene	C ₂ H ₄	g	-1411
buta-1,3-diene	C ₄ H ₆	g	-2541
ethyne	C ₂ H ₂	g	-1301
benzene	C ₆ H ₆	l	-3268
methylbenzene	C ₆ H ₅ CH ₃	l	-3910
naphthalene	C ₁₀ H ₈	s	-5156
chloroethane	C ₂ H ₅ Cl	g	-1413
iodoethane	C ₂ H ₅ I	l	-1463
trichloromethane	CHCl ₃	l	-473
methanol	CH ₃ OH	l	-726
ethanol	C ₂ H ₅ OH	l	-1367

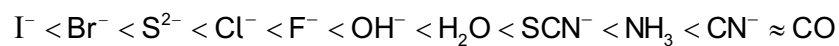
Substance	Formula	State	$\Delta H_c^\ominus$ (kJ mol ⁻¹)
propan-1-ol	C ₃ H ₇ OH	l	-2021
butan-1-ol	C ₄ H ₉ OH	l	-2676
cyclohexanol	C ₆ H ₁₁ OH	s	-3728
phenol	C ₆ H ₅ OH	s	-3053
ethoxyethane	(C ₂ H ₅) ₂ O	l	-2724
methanal	HCHO	g	-571
ethanal	CH ₃ CHO	g	-1167
benzaldehyde	C ₆ H ₅ CHO	l	-3525
propanone	(CH ₃) ₂ CO	l	-1790
pentan-3-one	(C ₂ H ₅) ₂ CO	l	-3100
phenylethanone	CH ₃ COC ₆ H ₅	l	-4149
methanoic acid	HCOOH	l	-255
ethanoic acid	CH ₃ COOH	l	-874
benzoic acid	C ₆ H ₅ COOH	s	-3228
ethanedioic acid	(COOH) ₂	s	-243
ethyl ethanoate	CH ₃ COOC ₂ H ₅	l	-2238
ethanamide	CH ₃ CONH ₂	s	-1186
methylamine	CH ₃ NH ₂	g	-1086
phenylamine	C ₆ H ₅ NH ₂	l	-3393
nitrobenzene	C ₆ H ₅ NO ₂	l	-3088
urea	CO(NH ₂) ₂	s	-633
glucose	C ₆ H ₁₂ O ₆	s	-2803
sucrose	C ₁₂ H ₂₂ O ₁₁	s	-5640

14. Common oxidation states of the 3d ions

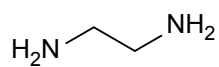
Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
								+1	
	+2	+2	+2	+2	+2	+2	+2	+2	+2
+3	+3	+3	+3	+3	+3	+3			
	+4	+4		+4					
		+5							
			+6	+6					
				+7					

15. Spectrochemical series

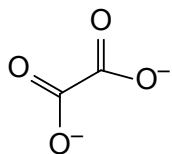
Ligands can be arranged in a spectrochemical series according to the energy difference they produce between the two sets of d-orbitals in an octahedral complex.



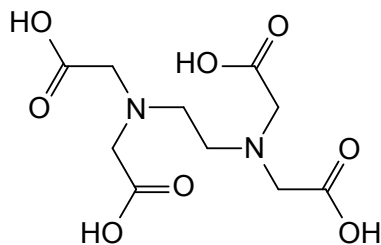
16. Ligands



1,2-ethanediamine

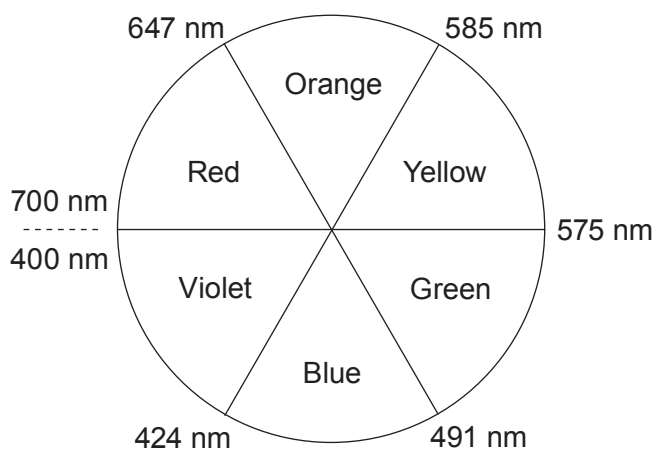


ethanedioate



EDTA

17. Colour wheel



18. Lattice enthalpies at 298 K (experimental values)

The lattice enthalpy values ($\Delta H_{\text{lattice}}^{\ominus}$) given relate to the endothermic process $M_aX_b(s) \rightarrow aM^{b+}(g) + bX^{a-}(g)$ in which the gaseous ions of a crystal are separated to an infinite distance from each other.

Experimental values

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

Alkali metal halides	$\Delta H_{\text{lattice}}^{\ominus} (\text{kJ mol}^{-1})$			
	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	$\Delta H_{\text{lattice}}^{\ominus} (\text{kJ mol}^{-1})$
CaF ₂	2651
BeCl ₂	3033
MgCl ₂	2540
CaCl ₂	2271
SrCl ₂	2170
BaCl ₂	2069
MgO	3791
CaO	3401

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

19. Enthalpies of aqueous solutions

Solute	$\Delta H_{\text{sol}}^{\ominus} (\text{kJ mol}^{-1})$	Solute	$\Delta H_{\text{sol}}^{\ominus} (\text{kJ mol}^{-1})$
NH_4Cl	+14.78	KCl	+17.22
NH_4NO_3	+25.69	KBr	+19.87
LiF	+4.73	KI	+20.33
LiCl	-37.03	RbF	-26.11
LiBr	-48.83	RbCl	+17.28
LiI	-63.30	RbBr	+21.88
NaF	+0.91	RbI	+25.10
NaCl	+3.88	CsF	-36.86
NaBr	-0.60	CsCl	+17.78
NaI	-7.53	CsBr	+25.98
KF	-17.73	CsI	+33.35

20. Enthalpies of hydration

Cations	$\Delta H_{\text{hyd}}^{\ominus} (\text{kJ mol}^{-1})$	Anions	$\Delta H_{\text{hyd}}^{\ominus} (\text{kJ mol}^{-1})$
Li^{+}	-538	F^{-}	-504
Na^{+}	-424	Cl^{-}	-359
K^{+}	-340	Br^{-}	-328
Rb^{+}	-315	I^{-}	-287
Cs^{+}	-291	ClO_3^{-}	-331
Be^{2+}	-2524	BrO_3^{-}	-358
Mg^{2+}	-1963	IO_3^{-}	-446
Ca^{2+}	-1616	ClO_4^{-}	-205
Sr^{2+}	-1483	OH^{-}	-519
Ba^{2+}	-1346	CN^{-}	-341
Ra^{2+}	-1335	NO_3^{-}	-316
Al^{3+}	-4741	HCO_3^{-}	-383
Ga^{3+}	-4745	CO_3^{2-}	-1486
In^{3+}	-4171	HSO_4^{-}	-362
Tl^{3+}	-4163	SO_4^{2-}	-1099
Tl^{+}	-346	PO_4^{3-}	-2921
Sn^{2+}	-1587		
Pb^{2+}	-1523		

21. Strengths of organic acids and bases

The acid strengths in the following tables are given in terms of 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	4.83
2-methylpropanoic	(CH ₃) ₂ CHCOOH	4.84
pentanoic	CH ₃ (CH ₂) ₃ COOH	4.83
2,2-dimethylpropanoic	(CH ₃) ₃ CCOOH	5.03
benzoic	C ₆ H ₅ COOH	4.20
phenylethanoic	C ₆ H ₅ CH ₂ COOH	4.31

Halogenated carboxylic acids

Name	Formula	pK_a
chloroethanoic	CH ₂ ClCOOH	2.87
dichloroethanoic	CHCl ₂ COOH	1.35
trichloroethanoic	CCl ₃ COOH	0.66
fluoroethanoic	CH ₂ FCOOH	2.59
bromoethanoic	CH ₂ BrCOOH	2.90
iodoethanoic	CH ₂ ICOOH	3.18

Phenols

Name	Formula	pK_a
phenol	C_6H_5OH	9.99
2-nitrophenol	$O_2NC_6H_4OH$	7.23
3-nitrophenol	$O_2NC_6H_4OH$	8.36
4-nitrophenol	$O_2NC_6H_4OH$	7.15
2,4-dinitrophenol	$(O_2N)_2C_6H_3OH$	4.07
2,4,6-trinitrophenol	$(O_2N)_3C_6H_2OH$	0.42

Alcohols

Name	Formula	pK_a
methanol	CH_3OH	15.5
ethanol	C_2H_5OH	15.5

Amines

Name	Formula	pK_b
ammonia	NH_3	4.75
methylamine	CH_3NH_2	3.34
ethylamine	$CH_3CH_2NH_2$	3.35
dimethylamine	$(CH_3)_2NH$	3.27
trimethylamine	$(CH_3)_3N$	4.20
diethylamine	$(C_2H_5)_2NH$	3.16
triethylamine	$(C_2H_5)_3N$	3.25
phenylamine	$C_6H_5NH_2$	9.13

22. Acid-base indicators

Indicator	pK_a	pH range	Colour change	
			Acid	Alkali
methyl orange	3.7	3.1–4.4	red	yellow
bromophenol blue	4.2	3.0–4.6	yellow	blue
bromocresol green	4.7	3.8–5.4	yellow	blue
methyl red	5.1	4.4–6.2	red	yellow
bromothymol blue	7.0	6.0–7.6	yellow	blue
phenol red	7.9	6.8–8.4	yellow	red
phenolphthalein	9.6	8.3–10.0	colourless	pink

23. Values of the ionization constant of water

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

24. Standard electrode potentials at 298 K

Oxidized species	⇌	Reduced species	$E^\ominus$ (V)
$\text{Li}^+(\text{aq}) + \text{e}^-$	⇌	$\text{Li}(\text{s})$	-3.04
$\text{K}^+(\text{aq}) + \text{e}^-$	⇌	$\text{K}(\text{s})$	-2.93
$\text{Ca}^{2+}(\text{aq}) + 2\text{e}^-$	⇌	$\text{Ca}(\text{s})$	-2.87
$\text{Na}^+(\text{aq}) + \text{e}^-$	⇌	$\text{Na}(\text{s})$	-2.71
$\text{Mg}^{2+}(\text{aq}) + 2\text{e}^-$	⇌	$\text{Mg}(\text{s})$	-2.37
$\text{Al}^{3+}(\text{aq}) + 3\text{e}^-$	⇌	$\text{Al}(\text{s})$	-1.66
$\text{Mn}^{2+}(\text{aq}) + 2\text{e}^-$	⇌	$\text{Mn}(\text{s})$	-1.18
$\text{H}_2\text{O}(\text{l}) + \text{e}^-$	⇌	$\frac{1}{2}\text{H}_2(\text{g}) + \text{OH}^-(\text{aq})$	-0.83
$\text{Zn}^{2+}(\text{aq}) + 2\text{e}^-$	⇌	$\text{Zn}(\text{s})$	-0.76
$\text{Fe}^{2+}(\text{aq}) + 2\text{e}^-$	⇌	$\text{Fe}(\text{s})$	-0.45
$\text{Ni}^{2+}(\text{aq}) + 2\text{e}^-$	⇌	$\text{Ni}(\text{s})$	-0.26
$\text{Sn}^{2+}(\text{aq}) + 2\text{e}^-$	⇌	$\text{Sn}(\text{s})$	-0.14
$\text{Pb}^{2+}(\text{aq}) + 2\text{e}^-$	⇌	$\text{Pb}(\text{s})$	-0.13
$\text{H}^+(\text{aq}) + \text{e}^-$	⇌	$\frac{1}{2}\text{H}_2(\text{g})$	0.00
$\text{Cu}^{2+}(\text{aq}) + \text{e}^-$	⇌	$\text{Cu}^+(\text{aq})$	+0.15
$\text{SO}_4^{2-}(\text{aq}) + 4\text{H}^+(\text{aq}) + 2\text{e}^-$	⇌	$\text{H}_2\text{SO}_3(\text{aq}) + \text{H}_2\text{O}(\text{l})$	+0.17
$\text{Cu}^{2+}(\text{aq}) + 2\text{e}^-$	⇌	$\text{Cu}(\text{s})$	+0.34
$\frac{1}{2}\text{O}_2(\text{g}) + \text{H}_2\text{O}(\text{l}) + 2\text{e}^-$	⇌	$2\text{OH}^-(\text{aq})$	+0.40
$\text{Cu}^+(\text{aq}) + \text{e}^-$	⇌	$\text{Cu}(\text{s})$	+0.52
$\frac{1}{2}\text{I}_2(\text{s}) + \text{e}^-$	⇌	$\text{I}^-(\text{aq})$	+0.54
$\text{Fe}^{3+}(\text{aq}) + \text{e}^-$	⇌	$\text{Fe}^{2+}(\text{aq})$	+0.77
$\text{Ag}^+(\text{aq}) + \text{e}^-$	⇌	$\text{Ag}(\text{s})$	+0.80
$\frac{1}{2}\text{Br}_2(\text{l}) + \text{e}^-$	⇌	$\text{Br}^-(\text{aq})$	+1.09
$\frac{1}{2}\text{O}_2(\text{g}) + 2\text{H}^+(\text{aq}) + 2\text{e}^-$	⇌	$\text{H}_2\text{O}(\text{l})$	+1.23
$\text{Cr}_2\text{O}_7^{2-}(\text{aq}) + 14\text{H}^+(\text{aq}) + 6\text{e}^-$	⇌	$2\text{Cr}^{3+}(\text{aq}) + 7\text{H}_2\text{O}(\text{l})$	+1.36
$\frac{1}{2}\text{Cl}_2(\text{g}) + \text{e}^-$	⇌	$\text{Cl}^-(\text{aq})$	+1.36
$\text{MnO}_4^-(\text{aq}) + 8\text{H}^+(\text{aq}) + 5\text{e}^-$	⇌	$\text{Mn}^{2+} + 4\text{H}_2\text{O}(\text{l})$	+1.51
$\frac{1}{2}\text{F}_2(\text{g}) + \text{e}^-$	⇌	$\text{F}^-(\text{aq})$	+2.87

25. Activity series

Increasing activity	
	
Li	
Cs	
Rb	
K	
Ba	
Sr	
Ca	
Na	
Mg	
Be	
Al	
C	
Zn	
Cr	
Fe	
Cd	
Co	
Ni	
Sn	
Pb	
H	
Sb	
As	
Bi	
Cu	
Ag	
Pd	
Hg	
Pt	
Au	

26. Infrared data

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

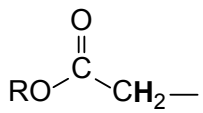
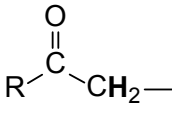
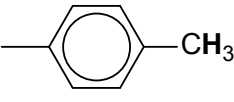
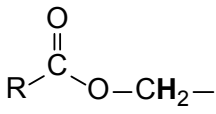
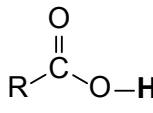
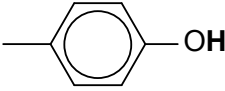
Bond	Organic molecules	Wavenumber (cm^{-1})	Intensity
C–I	iodoalkanes	490–620	strong
C–Br	bromoalkanes	500–600	strong
C–Cl	chloroalkanes	600–800	strong
C–F	fluoroalkanes	1000–1400	strong
C–O	alcohols, esters, ethers	1050–1410	strong
C=C	alkenes	1620–1680	medium-weak; multiple bands
C=O	aldehydes, ketones, carboxylic acids and esters	1700–1750	strong
C≡C	alkynes	2100–2260	variable
O–H	carboxylic acids (with hydrogen bonding)	2500–3000	strong, very broad
C–H	alkanes, alkenes, arenes	2850–3090	strong
O–H	alcohols and phenols (with hydrogen bonding)	3200–3600	strong, broad
N–H	primary amines	3300–3500	medium, two bands

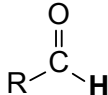
27. ^1H NMR data

Typical proton chemical shift values (δ) relative to tetramethylsilane (TMS) = 0 .

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

These values may vary in different solvents and conditions.

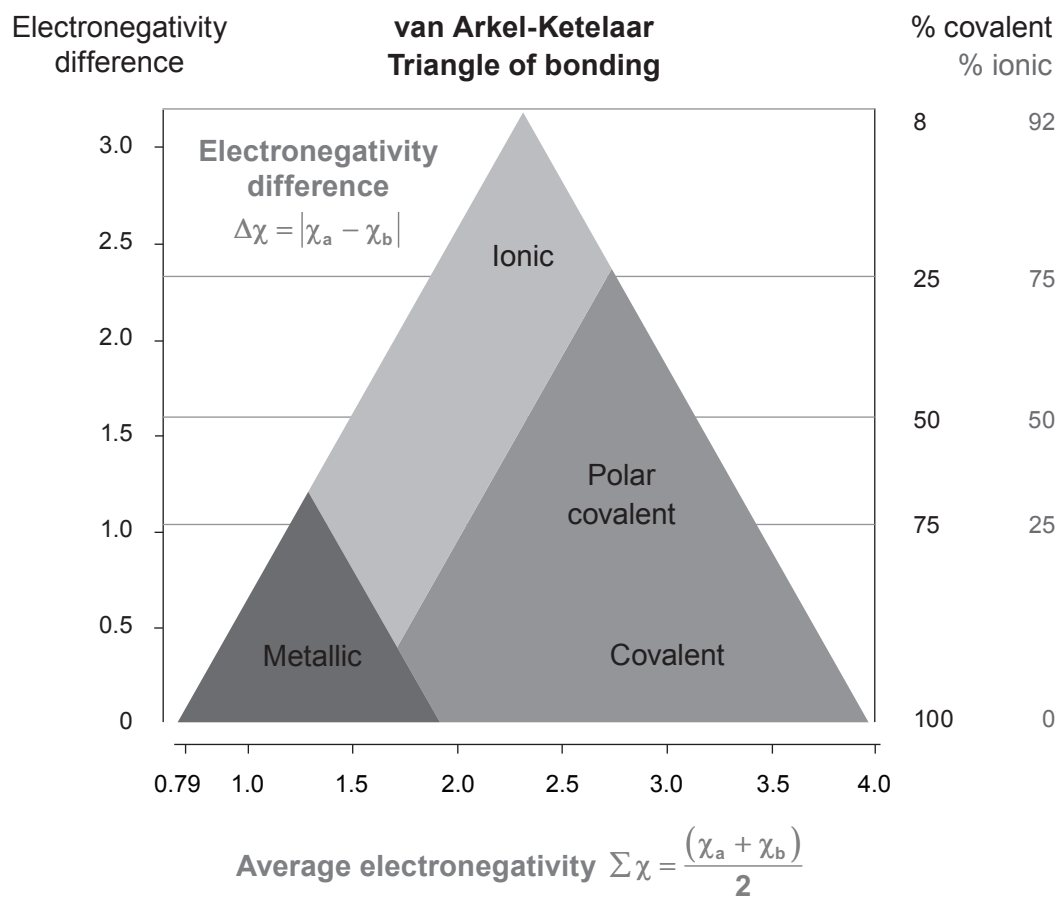
Type of proton	Chemical shift (ppm)
$-\text{CH}_3$	0.9–1.0
$-\text{CH}_2\text{R}$	1.3–1.4
$-\text{CHR}_2$	1.5
	2.0–2.5
	2.2–2.7
	2.5–3.5
$-\text{C}\equiv\text{C}-\text{H}$	1.8–3.1
$-\text{CH}_2-\text{Hal}$	3.5–4.4
$\text{R}-\text{O}-\text{CH}_2-$	3.3–3.7
	3.7–4.8
	9.0–13.0
$\text{R}-\text{O}-\text{H}$	1.0–6.0
$-\text{CH}=\text{CH}_2$	4.5–6.0
	4.0–12.0

Type of proton	Chemical shift (ppm)
	6.9–9.0
	9.4–10.0

28. Mass spectral fragments lost

Mass lost	Fragment lost
15	CH ₃
17	OH
18	H ₂ O
28	CH ₂ =CH ₂ , C=O
29	CH ₃ CH ₂ , CHO
31	CH ₃ O
45	COOH

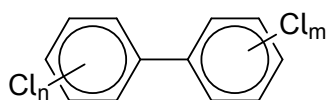
29. Triangular bonding diagram



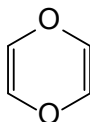
30. Resin identification codes

Resin Identification Code (RIC)	Plastic types	Resin Identification Code (RIC)	Plastic types
 PETE	polyethene terephthalate	 PP	polypropene
 HDPE	high-density polyethene	 PS	polystyrene
 PVC	polyvinyl chloride	 OTHER	other
 LDPE	low-density polyethene		

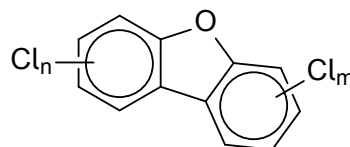
31. Representations of some materials molecules



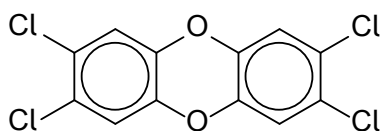
polychlorinated biphenyls



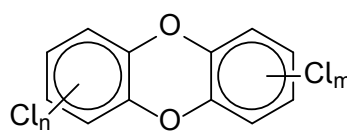
1,4-dioxin



polychlorinated dibenzofuran



2,3,7,8-tetrachlorodibenzodioxin

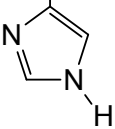


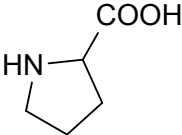
polychlorinated dibenzo-p-dioxin

32. Solubility product constants at 298 K

Compound	K_{sp}
BaCO_3	2.58×10^{-9}
$\text{Ba(OH)}_2 \cdot 8\text{H}_2\text{O}$	2.55×10^{-4}
BaSO_4	1.08×10^{-10}
CdCO_3	1.0×10^{-12}
Cd(OH)_2	7.2×10^{-15}
PbCO_3	7.40×10^{-14}
Pb(OH)_2	1.43×10^{-20}
PbSO_4	2.53×10^{-8}
Hg_2CO_3	3.6×10^{-17}
Hg_2SO_4	6.5×10^{-7}
NiCO_3	1.42×10^{-7}
Ni(OH)_2	5.48×10^{-16}
Ag_2CO_3	8.46×10^{-12}
Ag_2SO_4	1.20×10^{-5}
ZnCO_3	1.46×10^{-10}
Zn(OH)_2	3.0×10^{-17}

33. 2-amino acids

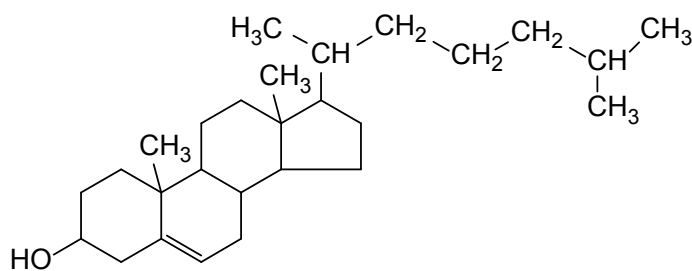
Common name	Symbol	Structural formula	pH of isoelectric point
alanine	Ala	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_3 \end{array}$	6.0
arginine	Arg	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{CH}_2-\text{CH}_2-\text{NH}-\text{C}-\text{NH}_2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

Common name	Symbol	Structural formula	pH of isoelectric point
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		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	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2 \\ \\ \text{C}_8\text{H}_6\text{N} \end{array}$	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

34. Lipids, carbohydrates and nucleotide components

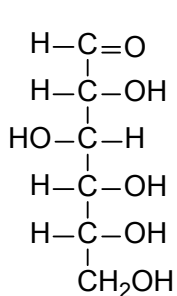
Lipids

Octanoic acid	$\text{CH}_3(\text{CH}_2)_6\text{COOH}$
Lauric acid	$\text{CH}_3(\text{CH}_2)_{10}\text{COOH}$
Palmitic acid	$\text{CH}_3(\text{CH}_2)_{14}\text{COOH}$
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	$\text{CH}_3(\text{CH}_2)_4(\text{CH}=\text{CHCH}_2)_2(\text{CH}_2)_6\text{COOH}$
α -Linolenic acid	$\text{CH}_3\text{CH}_2(\text{CH}=\text{CHCH}_2)_3(\text{CH}_2)_6\text{COOH}$

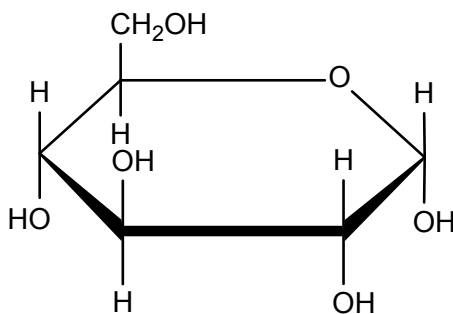


cholesterol

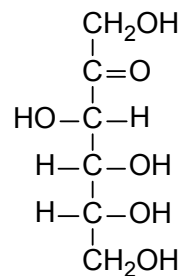
Carbohydrates



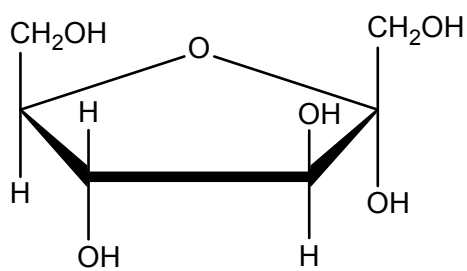
straight chain glucose



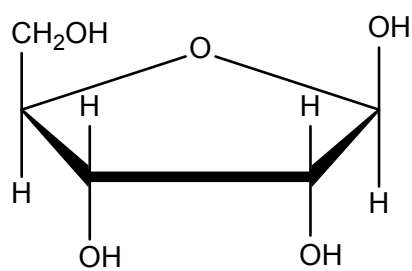
α -glucose



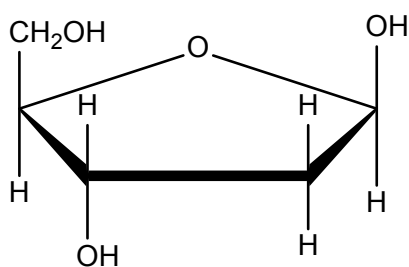
straight chain fructose



α -fructose

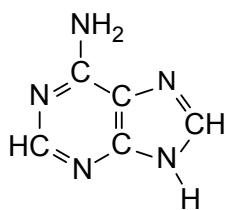


ribose

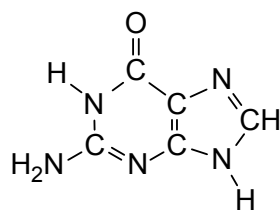


deoxyribose

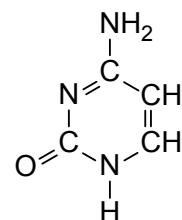
Nitrogenous bases



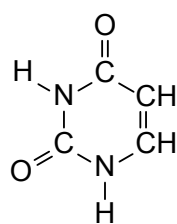
adenine



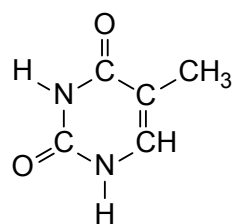
guanine



cytosine



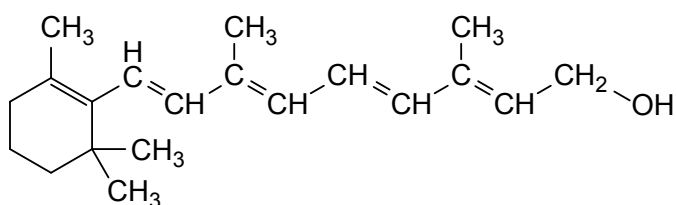
uracil



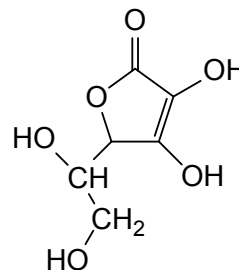
thymine

35. Vitamins and pigments

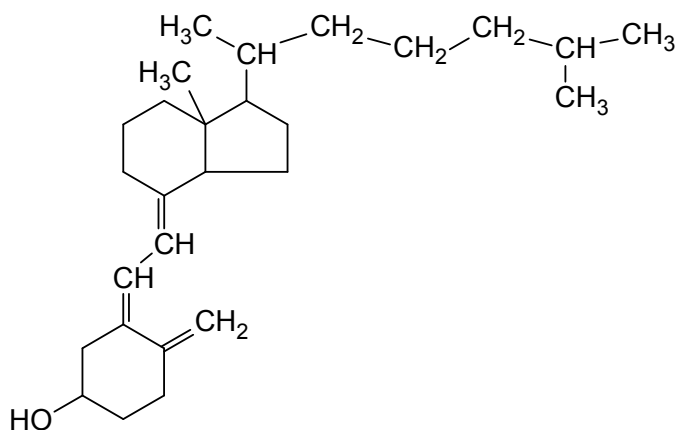
Vitamins



retinol (vitamin A)

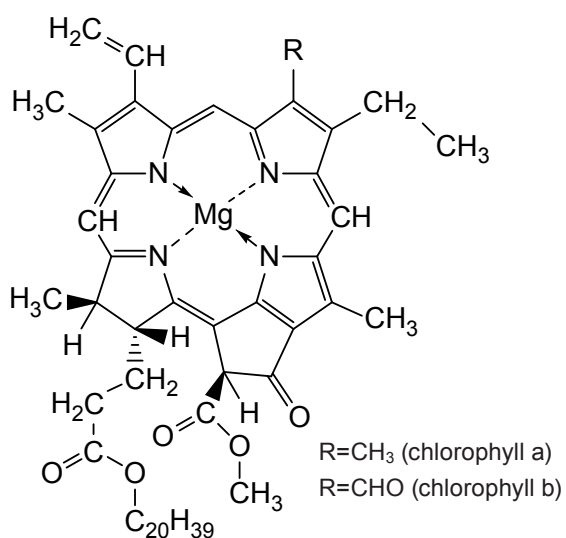


ascorbic acid (vitamin C)

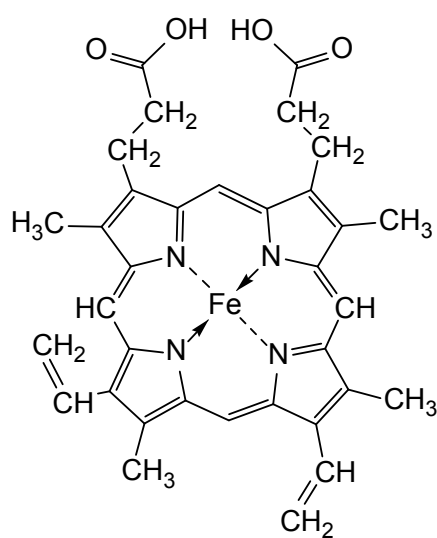


vitamin D (D₃)

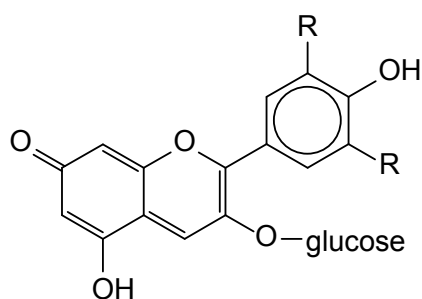
Pigments



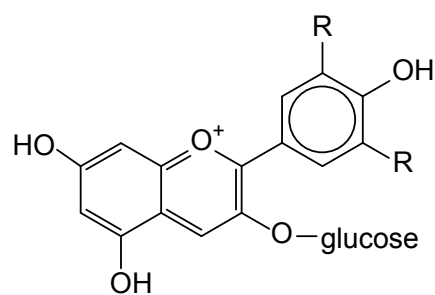
chlorophyll



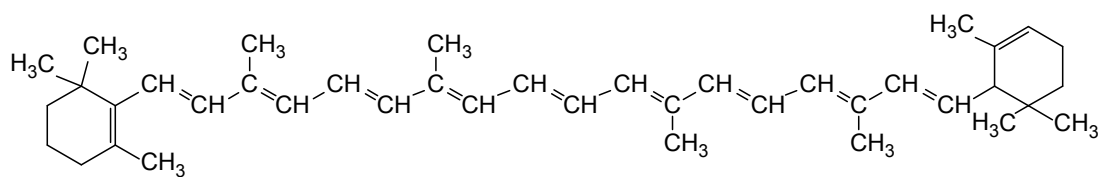
heme B



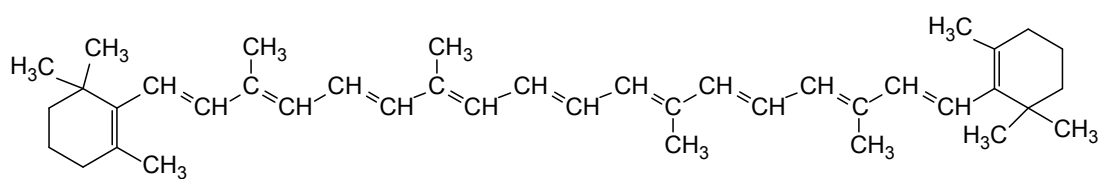
quinoidal base (blue)



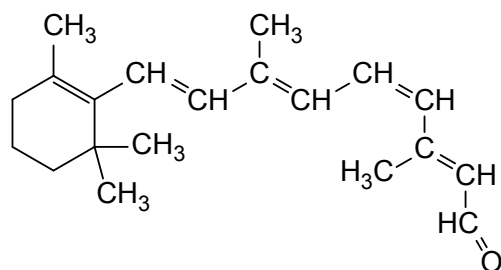
flavylum cation (red)



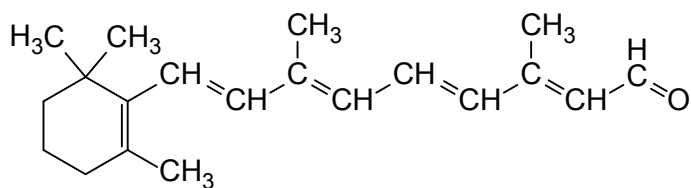
α -carotene



β -carotene

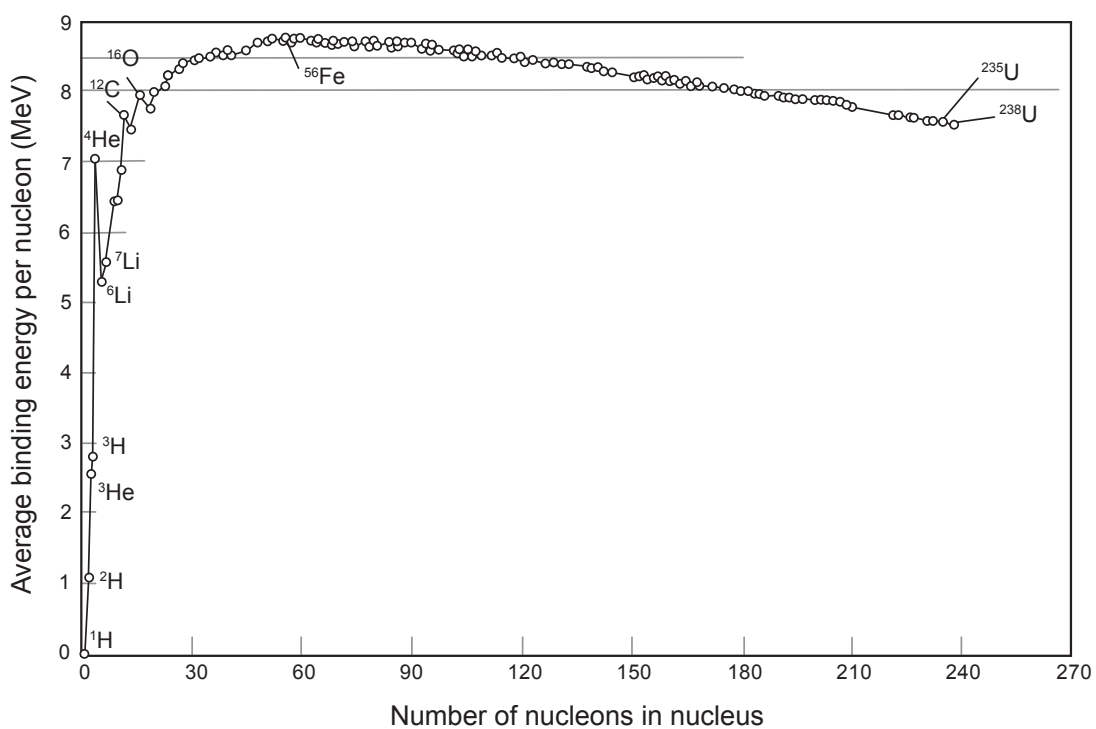


11-*cis*-retinal

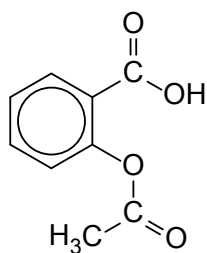


all-*trans*-retinal

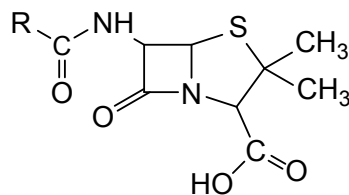
36. Binding energy curve



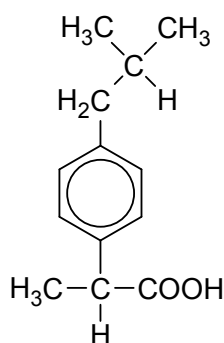
37. Representations of some medicinal molecules



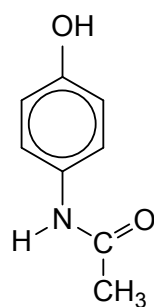
aspirin



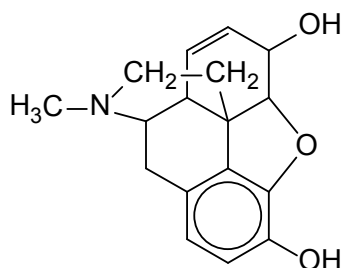
penicillin (general structure)



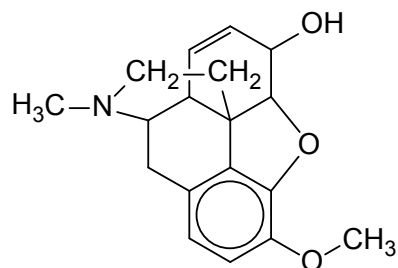
ibuprofen



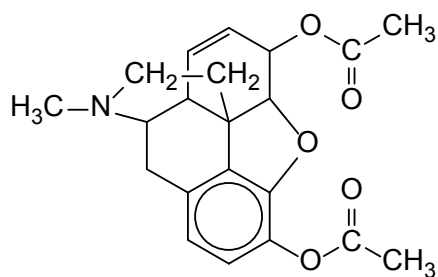
paracetamol (acetaminophen)



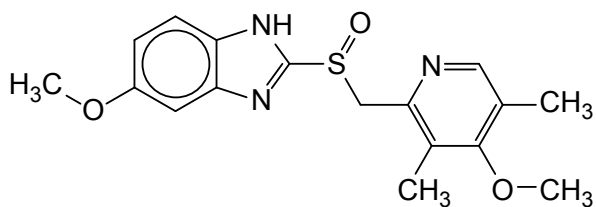
morphine



codeine



diamorphine (heroin)



omeprazole



38. References

Data in sections 9, 10, 11, 12, 13, 22, 26 and 27 was taken fully or in part from:

Aylward, G. and Findlay, T. 2008. *SI chemical data*. (5th edition). Queensland, Australia. John Wiley & Sons.

Data in section 20 reproduced by permission of The Royal Society of Chemistry.

Barret, J. 2003. *Inorganic chemistry in aqueous solution*. London, UK. Royal Society of Chemistry.

Data in section 13 was taken in part from:

Burgess, DR. 2012. "Thermochemical Data". *NIST Chemistry WebBook, NIST Standard Reference Database*. Number 69. <http://webbook.nist.gov>.

Data in sections 7, 8, 9, 12, 13, 18, 19, 21, 23, 24, 28, 32 and 33 was taken fully or in part from:

Haynes, WM. (ed). 2012. *CRC Handbook of chemistry and physics*. (93rd edition). Boca Raton, US. CRC Press.

Data in section 29 can be found in the following source:

Leach, MR. 2013. *Timeline of structural theory*. 04 January 2013. http://www.meta-synthesis.com/webbook/30_timeline/timeline.html.