

Chemistry data booklet

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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 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	$pH = -\log_{10} \left[H_3 O^+ \right]$ or $pH = -\log_{10} \left[H^+ \right]$
12.1	E = hv
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	% 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	$\log_{10}\frac{I_0}{I} = \varepsilon I c$

Topic	Equation
C.1	Energy density = $\frac{\text{energy released from fuel}}{\text{volume of fuel consumed}}$
C.1	Specific energy = energy released from fuel 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	$\frac{Rate_1}{Rate_2} = \sqrt{\frac{M_2}{M_1}}$
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 $STP = 2.27 \times 10^{-2} \text{ m}^3 \text{ mol}^{-1} = 22.7 \text{ dm}^3 \text{ mol}^{-1}$

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

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) = 6.63×10^{-34} J s

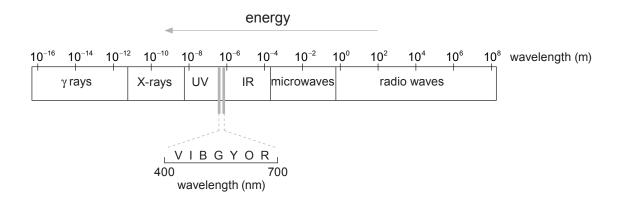
Faraday's constant (F) = 9.65×10^4 C mol⁻¹

lonic product constant for water (K_W) = 1.00 \times 10⁻¹⁴ mol² dm⁻⁶ at 298 K

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

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3. The electromagnetic spectrum



4. Fundamental particles

	Proton	Neutron	Electron
Mass (kg)	1.672622×10 ⁻²⁷	1.674927×10 ⁻²⁷	9.109383×10 ⁻³¹
Charge (C)	1.602189×10 ⁻¹⁹	0	1.602189×10 ⁻¹⁹

5. Names of the elements

Element	Symbol	Atomic number	Element	Symbol
actinium	Ac	89	dysprosium	Dy
aluminium	Al	13	einsteinium	Es
americium	Am	95	erbium	Er
antimony	Sb	51	europium	Eu
argon	Ar	18	fermium	Fm
arsenic	As	33	fluorine	ш
astatine	At	85	francium	Ā
barium	Ba	56	gadolinium	PS
berkelium	番	26	gallium	Ga
beryllium	Be	4	germanium	Ge
bismuth	Bi	83	plog	Au
bohrium	Bh	107	hafnium	눈
boron	В	5	hassium	SH.
bromine	Br	35	helium	He
cadmium	Cd	48	holmium	Н
caesium	S	55	hydrogen	エ
calcium	Ca	20	indium	In
californium	Ç	86	iodine	Ι
carbon	၁	9	iridium	Ir
cerium	Ce	58	iron	Fe
chlorine	ರ	17	krypton	Ā
chromium	Ç	24	lanthanum	La
cobalt	Co	27	lawrencium	٦
copernicium	Cn	112	lead	Pb
copper	Cu	29	lithium	ij
curium	Cm	96	lutetium	Γn
darmstadtium	Ds	110	magnesium	Mg
dubnium	Db	105	manganese	Mn

Element	Symbol	Atomic number	Element	Symbol	Atomic number
meitnerium	Mt	109	ruthenium	Ru	44
mendelevium	Md	101	rutherfordium	Rf	104
mercury	Hg	80	samarium	Sm	62
molybdenum	Mo	42	scandium	Sc	21
neodymium	Nd	09	seaborgium	Sg	106
neon	Ne	10	selenium	Se	34
neptunium	Np	93	silicon	Si	14
nickel	Z	28	silver	Ag	47
niobium	qN	41	sodium	Na	11
nitrogen	Z	7	strontium	Sr	38
nobelium	No	102	sulfur	S	16
osmium	SO	92	tantalum	Та	23
oxygen	0	8	technetium	Tc	43
palladium	Pd	46	tellurium	Те	52
phosphorus	Д	15	terbium	qL	99
platinum	Pt	78	thallium	1L	81
plutonium	Pu	94	thorium	Th	06
polonium	Po	84	thulium	шL	69
potassium	Х	19	tin	Sn	20
praseodymium	Pr	59	titanium	Ti	22
promethium	Pm	61	tungsten	W	74
protactinium	Ра	91	uranium	N	92
radium	Ra	88	vanadium	Λ	23
radon	Rn	98	xenon	Xe	54
rhenium	Re	75	ytterbium	q,	02
rhodium	Rh	45	yttrium	Ь	39
roentgenium	Rg	111	zinc	Zn	30
rubidium	Rb	37	zirconium	Zr	40

6. The periodic table

				1	1		
8	2 He	10 Ne 20.18	18 Ar 39.95	36 7	54 Xe 131.29	86 Rn (222)	118 Uuo (294)
17		9 F 19.00	17 CI 35.45	35 Br	53 I 126.90	85 At (210)	117 Uus (294)
16		8 O 16.00	16 S 32.07	% % %	52 Te 127.60	84 Po (209)	116 Uuh (293)
15		7 N 14.01	15 P 30.97	33 AS	51 Sb 121.76	83 Bi 208.98	115 Uup (288)
4		6 12.01	14 Si 28.09	32 Ge	50 Sn 118.71	82 Pb 207.20	114 Uuq (289)
13		5 B 10.81	13 Al 26.98	31 Ga	49 In 114.82	81 Tl 204.38	113 Uut (286)
12				30 Zn	_		
7				29 Cu			
10				28 E 860		78 Pt 195.08	
6				27 Co	 		
∞	nber 1t	omic		26 Fe			108 Hs (269)
7	Atomic number Element	Relative atomic mass			(98)	,	
					Mo 95.96		
9						`	
ß					44 Nb 92.91	`	
4				22 1	40 Ar 91.22	72 Hf 178.49	104 Rf (267)
က				21 Sc	39 > 88.91	57 † La 138.91	89 ‡ Ac (227)
7		4 Be 9.01	12 Mg 24.31	20 Ca	38 Sr 87.62	56 Ba 137.33	88 Ra (226)
-	- I	3 Li 6.94	11 Na 22.99	19 7 × 19	37 Rb 85.47	55 Cs 132.91	87 Fr (223)
	_	7	က	4	5	9	

	28	26	09	61	62	63	49	92	99	29	89	69	20	71
+	Ce	Ą	o Z	Pm	Sm	Ē	ည်	Д	٥	유	ш	E	χ	Ľ
	140.12	140.91	144.24	(145)	150.36	151.96	157.25	158.93	162.50	164.93	167.26	168.93	173.05	174.97
	06	91	92	93	94	92	96	26	86	66	100	101	102	103
++	۲ ۲	Ъа	-	d N	Pu	Am	CH	ᄶ	ჯ	Es	F	Σ	8	בֿ
	232.04	232.04 231.04	238.03	(237)	(244)	(243)	(247)	(247)	(251)	(252)	(257)	(258)	(528)	(262)

7. Melting points and boiling points of the elements (at 101.325 kPa)

-259.2 H						Melting po	ng point (°C)										Ī
252.9						i	•										-268.9
80.5	1287	_				Element	ent					2077	3500	-210.0	-218 B	-2197	-248 6
5.	2											5 1	200	2.5	5.	1	5
_	Be					od pailing	()°/ taioa 5a					ω	ပ	z	0	ш	o N
1342	2468					אל פווווסם	()					4000	4827	-195.8	-183.0	-188.1	-246.0
7.79	650.0										•	660.3	1414	44.15	115.2	-101.5	-189.3
Na	M											₹	S	Δ.	ဟ	ರ	Ā
82.9	1090											2519	3265	280.5	444.6	-34.04	-185.8
3.38	842.0	1541	1670	1910	1907	1246	1538	1495	1455	1085	419.5	29.77	938.2	816.8	220.8	-7.050	-157.4
¥	Ca	သွ	j	>	ပ်	Ş	Ъ	ပိ	Z	D C	Zu	Ga	ge	As	Se	ğ	ž
758.8	1484	2836	3287	3407	2671	2061	2861	2927	2913	2560	0.706	2229	2833	613.0	684.8	58.78	-153.4
9.30	768.8	1522	1854	2477	2622	2157	2333	1963	1555	961.8	321.1	156.6	231.9	9.069	449.5	113.7	-111.8
Rb	Š	>	Ż	g	õ	ည	Ru	몺	Pd	Ag	ဦ	П	Sn	Sp	Ъ	Ι	Xe
87.8	1377	3345	4406	4741	4639	4262	4147	3692	2963	2162	8.992	2027	2586	1587	8.786	184.4	-108.1
8.44	725.0	920.0	2233	3017	3414	3453	3033	2446	1768	1064	-38.83	303.8	327.5	271.4	253.8	301.8	-71.15
Cs	Ва	La	¥	ā	>	Re	ő	<u>_</u>	풉	Ρn	Ĕ	F	P	洒	Ъ	¥	R
8.02	1845	3464	4600	5455	5555	2900	2008	4428	3825	2836	356.6	1473	1749	1564	962.0	336.8	-61.85
7.00	8.669	1050															
Ŧ	Ra	Ac															
8.92	1140	3200															

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

																1		
2372 He	2081	Ne		1520	Ā		1351	궃		1170	×	2.6	1037	R				
	1681 -328	ш	4.0	1251 -349	៊	3.2	1140 -325	Ŗ	3.0	1008 -295	П	2.7	-270 1037	¥	2.2			
	1314 -141	0	3.4	1000 -200	g G G	2.6	-78 941 -195	Se	2.6	869 -190	Te	2.1	-91 812 -183	Ъ	2.0			
	1402	z	3.0	1012 -72	۵	2.2	944	As	2.2	831 -101	Sb	2.0	703	Ö	1.9			
	-27 1086 -122	ပ	2.6	-42 787 -134	Si	1.9	762 -119	g	2.0	709 -107	Sn	2.0	716 -35	Pb	6 .			
	801 -27	ω	2.0	578 -42	¥	1.6	57941	Ga	1.8	258 –29	In	1.8	589 -36 716	F	1.8			
							906	Z	1.6	898	D C	1.7	1007	Hg	1.9			
							745 -119	D C	6.1	731 -126	Ag	0.0	890223	Αn	2.4			
				-			-64 737 -112 745 -119	ź	6.1	80454	Pd	2.2	-151 864 -205 890	¥	2.2			
in affinity (kJ mol ⁻¹) (2nd EA / kJ mol ⁻¹)							-15 760 -64	ပိ	1.9	720 -110	Rh	2.3	865 -151	ŀ	2.2			
Electron affinity (kJ mol ⁻¹) (2nd EA / kJ mol ⁻¹)			vity				762 -15	Fe	1.8	710 -101	Ru	2.2	-14 814 -106 865	SO	2.2			
Electr	Element		Electronegati vity				717	M	9.1	702 -53	٦c	2.1		Re	1.9			
ation J mol ⁻¹)			Ele				-51 653 -64 717	ပ်	1.7	684 -72 702	Mo	2.2	-1 728 -31 759 -79 756	>	1.7			
First ionization energy (kJ mol ⁻¹)							651	>	1.6	652 -88 684	Q N	1.6	72831	Та	1.5			
							-18 6598	F	1.5	-30 640 -41	Zr	1.3	-45 659 -1	Ħ	1.3			
							633	Sc	4.	-5 600 -30	>	1.2		La	7.	499 –34	Ac	1.1
	006	Be	9.1	738	Mg	ر. نی	-2	Ca	1.0		S	1.0	-46 503 -14 538	Ва	6.0	509 -10 499	Ra	6.0
1312 –73 H 2.2	520 -60 900	=	1.0	496 -53 738	Na	6.0	419 -48 590	×	0.8	403 -47 549	Rb	0.8	376 -46	S	0.8	393 -47 509	ŗ	0.7

9. Atomic and ionic radii of the elements

37 Re 62 Ne 62	101 Ar	116 Kr		136 Xe		146 Rn		
60 F 133 (1–)	100 CI 181 (1-)	117 Br	196 (1–)	136 I	220 (1-)	148 At	!	
-	104 100 S CI 184 (2-) 181 (1-)	118 Se	198 (2-)	137 Te	221 (2-)	142 Po	97 (4+)	
7	109 P 38 (5+	120 As	58 (3+ 46 (5+	140 Sb	76 (3+)	150 Bi	103 (3+) 76 (5+)	
75 C 16 (4+)	114 Si 40 (4+)	120 Ge	53 (4+) 272 (4-)	140 Sn	118 (2+) 69 (4+)	145 Pb	119 (2+) 78 (4+)	
84 B 27 (3+)	124 Al 54 (3+)	123 Ga	62 (3+)	142 In	80 (3+)	<u>4</u> ⊢	150 (1+) 89 (3+)	
		120 Zn	(4 (2+)	140 Cd	95 (2+)		119 (1+) 102 (2+)	
		122 Cu	73 (2+)	136 Ag	115 (1+)	130 Au	137 (1+) 85 (3+)	
		117 Ni				130 P	80 (2+) 63 (4+)	
		118 Co	65 (2+) 55 (3+)	134 Rh	67 (3+) 60 (4+)	132 F	68 (3+) 63 (4+)	
radius 2 m)		124 Fe				136 Q	63 (4+) 55 (6+)	
Atomic radius (10 ⁻¹² m) Element lonic radius (10 ⁻¹² m)		129 Mn	83 (2+) 53 (4+)	138 Tc	65 (4+)	141 Re	63 (4+) 53 (7+)	
	•	130 Cr				150 X	66 (4+) 60 (6+)	
		> > (79 (2+) 54 (5+)	156 Nb	72 (3+) 64 (5+)	158 7.	64 (5+)	
		148 Ti				25 7		
		159 SC	(2 (3+)	176 Y	90 (3+)	46 –	103 (3+)	201 Ac
99 Be 45 (2+)	140 Mg 72 (2+)	200 174 Ca	100 (2+)	190 Sr	18 (2+)	206 Ba	35 (2+)	211 Ra
32 H 130 Li 76 (1+)	160 Na 102 (1+)	200 X	138 (1+)	215 Rb	152 (1+)	238 Cs	167 (1+) 1	242 Fr

10. Covalent bond lengths

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

	Br	С	Cl	F	Н	I	N	0	Р	S	Si
Br	228	194	214	176	141	247	214		220	227	216
С	194	154	177	138	108	214	147	143	184	182	185
Cl	214	177	199	163	128	232	197	170	203	199	202
F	176	138	163	142	92	257	136	142	154	158	156
Н	141	108	128	92	74	160	101	97	142	134	148
I	247	214	232	257	160	267			247		243
N	214	147	197	136	101		146	136		175	174
0		143	170	142	97		136	148	154	161	163
Р	220	184	203	154	142	247		154	221	210	
S	227	182	199	158	134		175	161	210	205	215
Si	216	185	202	156	148	243	174	163		215	232

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

C=C 134	C≡N 1	116 N	≡N 110	
C≡C 120	C=O 1	122 N	=O 114	
C=C 140 (in benzene)	C=S 1	156 O	=O 121	
C=N 130	N=N 1	125 S	=S 189	

11. Bond enthalpies and average bond enthalpies at 298 K

Single bonds (kJ mol⁻¹)

	Br	С	Cl	F	Н	I	N	0	Р	S	Si
Br	193	285	219	249	366	178		201	264	218	330
С	285	346	324	492	414	228	286	358	264	289	307
Cl	219	324	242	255	431	211	192	206	322	271	400
F	249	492	255	159	567	280	278	191	490	327	597
Н	366	414	431	567	436	298	391	463	322	364	323
I	178	228	211	280	298	151		201	184		234
N		286	192	278	391		158	214			
0	201	358	206	191	463	201	214	144	363		466
Р	264	264	322	490	322	184		363	198		
S	218	289	271	327	364					266	293
Si	330	307	400	597	323	234		466		293	226

Multiple bonds (kJ mol⁻¹)

C=C 614	C≡N 890	N≡N 945
C≡C 839	C=O 804	N=O 587
C=C 507 (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	∆H [⊖] _f (kJ mol⁻¹)	∆G [⊖] (kJ mol⁻¹)	S [⊕] (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	C₄H 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	НСООН	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 (ΔH_c°) in the following table refer to a temperature of 298 K and a pressure of 1.00×10^5 Pa.

Substance	Formula	State	$\Delta H_{\rm c}^{\ominus}({ m kJmol}^{-1})$	Substance	Formula	State	$\Delta H_{\rm c}^{\oplus}$ (kJ mol ⁻¹)
hydrogen	H ²	D	-286	propan-1-ol	С ₃ Н ₇ ОН	_	-2021
sulfur	S	S	-297	butan-1-ol	C₄H ₃ OH	1	-2676
carbon (graphite)	O	S	-394	cyclohexanol	С ₆ Н ₁ ОН	S	-3728
carbon monoxide	00	D	-283	phenol	Сеньон	S	-3053
methane	CH ₄	D	-891	ethoxyethane	$(C_2H_5)_2O$	_	-2724
ethane	C ₂ H ₆	D	-1561	methanal	НСНО	ס	-571
propane	C ₃ H ₈	D	-2219	ethanal	СН³СНО	ס	-1167
butane	C₄H₁₀	D	-2878	benzaldehyde	СенсСНО	1	-3525
pentane	C ₅ H ₁₂	_	-3509	propanone	(CH ₃) ₂ CO	_	-1790
hexane	C ₆ H ₁₄	_	-4163	pentan-3-one	(C ₂ H ₅) ₂ CO	_	-3100
octane	C ₈ H ₁₈	_	-5470	phenylethanone	CH ₃ COC ₆ H ₅	_	-4149
cyclohexane	C ₆ H ₁₂	_	-3920	methanoic acid	НСООН	_	-255
ethene	C_2H_4	D	-1411	ethanoic acid	СН3СООН	_	-874
buta-1,3-diene	C₄H ₆	D	-2541	benzoic acid	С _в Н _с СООН	S	-3228
ethyne	C_2H_2	D	-1301	ethanedioic acid	(COOH) ₂	S	-243
benzene	C ₆ H ₆	1	-3268	ethyl ethanoate	CH ₃ COOC ₂ H ₅	1	-2238
methylbenzene	C ₆ H ₅ CH ₃	1	-3910	ethanamide	CH ₃ CONH ₂	S	-1186
naphthalene	C ₁₀ H ₈	S	-5156	methylamine	CH ₃ NH ₂	б	-1086
chloroethane	C ₂ H ₅ Cl	б	-1413	phenylamine	$C_6H_5NH_2$	1	-3393
iodoethane	C ₂ H ₅ I	1	-1463	nitrobenzene	$C_6H_5NO_2$	1	-3088
trichloromethane	CHCl³	1	-473	urea	$CO(NH_2)_2$	S	-633
methanol	СН³ОН	1	-726	glucose	$C_6H_2O_6$	S	-2803
ethanol	C ₂ H ₅ OH	1	-1367	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.

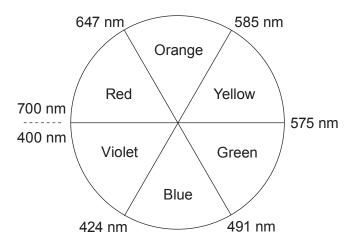
$$I^- < Br^- < S^{2-} < Cl^- < F^- < OH^- < H_2O < SCN^- < NH_3 < CN^- \approx CO$$

16. Ligands

EDTA

17. Colour wheel

ethanedioate



18. Lattice enthalpies at 298 K (experimental values)

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

Experimental values

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

Alkali metal halides	$\Delta oldsymbol{\mathcal{H}}_{ ext{lattice}}^{\ominus} ext{(kJ mol}^{-1} ext{)}$							
	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	$\Delta oldsymbol{\mathcal{H}}^\ominus_{ ext{lattice}}$ (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	Δ H [⊖] _{lattice} (kJ mol ⁻¹)
SrO	3223
ВаО	3054
CuCl ₂	2824
AgF	974
AgCl	918
AgBr	905
AgI	892

19. Enthalpies of aqueous solutions

Solute	$\Delta H_{\rm sol}^{\ominus}$ (kJ mol ⁻¹)
NH₄Cl	+14.78
NH ₄ NO ₃	+25.69
LiF	+4.73
LiCl	-37.03
LiBr	-48.83
LiI	-63.30
NaF	+0.91
NaCl	+3.88
NaBr	-0.60
NaI	- 7.53
KF	-17.73

Solute	$\Delta H_{\rm sol}^{\ominus}$ (kJ mol ⁻¹)
KCl	+17.22
KBr	+19.87
KI	+20.33
RbF	-26.11
RbCl	+17.28
RbBr	+21.88
RbI	+25.10
CsF	-36.86
CsCl	+17.78
CsBr	+25.98
CsI	+33.35

20. Enthalpies of hydration

Cations	Δ H [⊕] _{hyd} (kJ mol ⁻¹)
Li ⁺	-538
Na ⁺	-424
K ⁺	-340
Rb ⁺	- 315
Cs ⁺	-291
Be ²⁺	-2524
Mg ²⁺	-1963
Ca ²⁺	-1616
Sr ²⁺	-1483
Ba ²⁺	-1346
Ra ²⁺	-1335
Al ³⁺	-4741
Ga³+	-4745
In ³⁺	-4171
Tl ³⁺	-4163
Tl ⁺	-346
Sn ²⁺	-1587
Pb ²⁺	-1523

Anions	∆H _{hyd} (kJ mol ⁻¹)
F ⁻	-504
Cl ⁻	-359
Br^-	-328
I ⁻	-287
ClO_3^-	-331
BrO_3^-	-358
IO_3^-	-446
ClO^4	-205
OH^-	-519
CN ⁻	-341
NO_3^-	-316
HCO^3	-383
CO_3^{2-}	-1486
HSO^4	-362
SO ₄ ²⁻	-1099
PO ₄ ³⁻	-2921

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	p <i>K</i> _a
methanoic	нсоон	3.75
ethanoic	CH₃COOH	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 H₅COOH	4.20
phenylethanoic	C ₆ H ₅ CH ₂ COOH	4.31

Halogenated carboxylic acids

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

Phenols

Name	Formula	p <i>K</i> _a
phenol	C ₆ H ₅ OH	9.99
2-nitrophenol	O ₂ NC ₆ H ₄ OH	7.23
3-nitrophenol	O ₂ NC ₆ H ₄ OH	8.36
4-nitrophenol	O ₂ NC ₆ H ₄ OH	7.15
2,4-dinitrophenol	$(O_2N)_2C_6H_3OH$	4.07
2,4,6-trinitrophenol	(O ₂ N) ₃ C ₆ H ₂ OH	0.42

Alcohols

Name	Formula	p <i>K</i> _a
methanol	CH ₃ OH	15.5
ethanol	C ₂ H ₅ OH	15.5

Amines

Name	Formula	р <i>К</i> _ь
ammonia	NH ₃	4.75
methylamine	CH ₃ NH ₂	3.34
ethylamine	CH ₃ CH ₂ NH ₂	3.35
dimethylamine	(CH ₃) ₂ NH	3.27
trimethylamine	(CH ₃) ₃ N	4.20
diethylamine	$(C_2H_5)_2NH$	3.16
triethylamine	$(C_2H_5)_3N$	3.25
phenylamine	C ₆ H ₅ NH ₂	9.13

22. Acid-base indicators

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

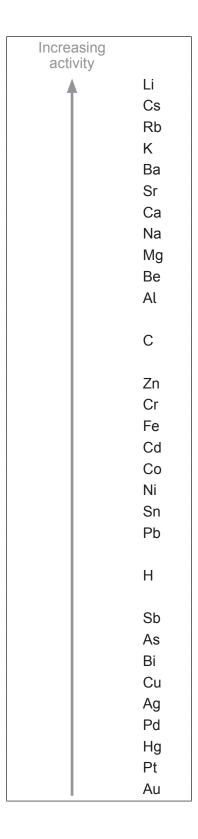
23. Values of the ionization constant of water

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	<i>E</i> [⊕] (V)
Li ⁺ (aq) + e ⁻		Li(s)	-3.04
K ⁺ (aq) + e ⁻		K(s)	-2.93
Ca ²⁺ (aq) + 2e ⁻		Ca(s)	-2.87
Na ⁺ (aq) + e ⁻		Na(s)	-2.71
Mg ²⁺ (aq) + 2e ⁻		Mg(s)	-2.37
Al ³⁺ (aq)+3e ⁻		Al(s)	-1.66
Mn ²⁺ (aq) + 2e ⁻		Mn(s)	-1.18
$H_2O(l)+e^-$		$\frac{1}{2}H_2(g) + OH^-(aq)$	-0.83
Zn ²⁺ (aq) + 2e ⁻		Zn(s)	-0.76
Fe ²⁺ (aq) + 2e ⁻		Fe(s)	-0.45
Ni ²⁺ (aq) + 2e ⁻		Ni(s)	-0.26
Sn ²⁺ (aq) + 2e ⁻		Sn(s)	-0.14
Pb ²⁺ (aq) + 2e ⁻		Pb(s)	-0.13
H ⁺ (aq) + e ⁻		$\frac{1}{2}H_2(g)$	0.00
Cu ²⁺ (aq) + e ⁻		Cu ⁺ (aq)	+0.15
SO ₄ ²⁻ (aq) + 4H ⁺ (aq) + 2e ⁻		$H_2SO_3(aq) + H_2O(l)$	+0.17
Cu ²⁺ (aq) + 2e ⁻		Cu(s)	+0.34
$\frac{1}{2}$ O ₂ (g) + H ₂ O(l) + 2e ⁻		2OH⁻(aq)	+0.40
Cu ⁺ (aq)+e ⁻		Cu(s)	+0.52
$\frac{1}{2}I_{2}(s)+e^{-}$		$\mathrm{I}^{\scriptscriptstyle{-}}(aq)$	+0.54
Fe ³⁺ (aq) + e ⁻		Fe ²⁺ (aq)	+0.77
Ag ⁺ (aq) + e ⁻		Ag(s)	+0.80
$\frac{1}{2} Br_2(l) + e^-$		Br ⁻ (aq)	+1.09
$\frac{1}{2}O_2(g) + 2H^+(aq) + 2e^-$		$H_2O(l)$	+1.23
$Cr_2O_7^{2-}(aq) + 14H^+(aq) + 6e^-$		$2Cr^{3+}(aq) + 7H_2O(l)$	+1.36
$\frac{1}{2}\operatorname{Cl}_{2}(g) + e^{-}$		Cl ⁻ (aq)	+1.36
$MnO_4^-(aq) + 8H^+(aq) + 5e^-$		$Mn^{2+} + 4H_2O(l)$	+1.51
$\frac{1}{2}F_{2}(g) + e^{-}$		F ⁻ (aq)	+2.87

25. Activity series



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	200-600	strong
C-C	chloroalkanes	600–800	strong
C-F	fluoroalkanes	1000–1400	strong
0-0	alcohols, esters, ethers	1050–1410	strong
O=0	alkenes	1620–1680	medium-weak; multiple bands
0=0	aldehydes, ketones, carboxylic acids and esters	1700–1750	strong
C≡C	alkynes	2100–2260	variable
H-0	carboxylic acids (with hydrogen bonding)	2500-3000	strong, very broad
C-H	alkanes, alkenes	2850-3090	strong
H-0	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.

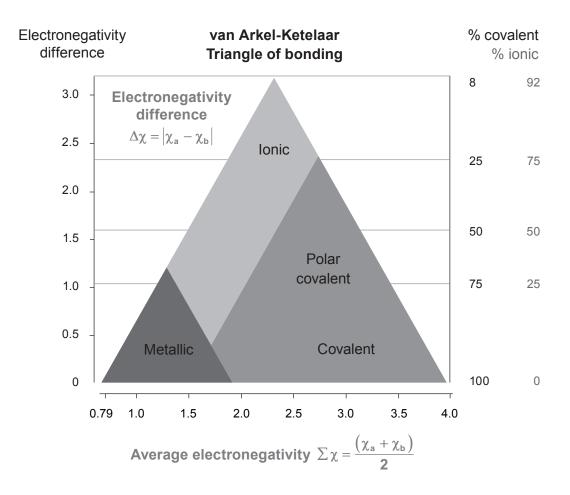
Type of proton	Chemical shift (ppm)
—C H ₃	0.9–1.0
—C H ₂ R	1.3–1.4
—C H R ₂	1.5
$^{\circ}_{RO}^{\circ}_{C}$ C H $_2$ —	2.0–2.5
$^{\circ}_{R}^{\circ}_{C}$ C H ₂ —	2.2–2.7
——————————————————————————————————————	2.5–3.5
—C≡C −H	1.8–3.1
—C H ₂ -Hal	3.5-4.4
R-O-C H ₂ -	3.3–3.7
$ \begin{array}{c} O \\ \parallel \\ C \\ O-C\mathbf{H}_2- \end{array} $	3.7–4.8
O 	9.0–13.0
R-O- H	1.0-6.0
—СН=С Н ₂	4.5-6.0
——ОН	4.0–12.0

Type of proton	Chemical shift (ppm)	
————	6.9–9.0	
O C H	9.4–10.0	

28. Mass spectral fragments lost

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

29. Triangular bonding diagram



30. Resin identification codes

Resin Identification Code (RIC)	Plastic types
PETE	polyethene terephthalate
2 HDPE	high-density polyethene
PVC	polyvinyl chloride
LDPE	low-density polyethene

Resin Identification Code (RIC)	Plastic types
5 PP	polypropene
6 PS	polystyrene
OTHER	other

31. Representations of some materials molecules

polychlorinated biphenyls

$$\binom{0}{0}$$

1,4-dioxin

$$Cl_n$$
 Cl_m

polychlorinated dibenzofuran

2,3,7,8-tetrachlorodibenzodioxin

$$Cl_m$$
 Cl_m

polychlorinated dibenzo-p-dioxin

32. Solubility product constants at 298 K

Compound	K _{sp}	
BaCO ₃	2.58×10 ⁻⁹	
Ba(OH) ₂ . 8H ₂ 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 ₂ CO ₃	3.6×10 ⁻¹⁷	
Hg ₂ SO ₄	6.5×10 ⁻⁷	
NiCO ₃	1.42×10 ⁻⁷	
Ni(OH) ₂	5.48×10 ⁻¹⁶	
Ag ₂ CO ₃	8.46×10 ⁻¹²	
Ag ₂ SO 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	H₂N—CH—COOH CH₃	6.0
arginine	Arg	H ₂ N-CH-COOH CH ₂ -CH ₂ -CH ₂ -NH-C-NH ₂ NH	10.8
asparagine	Asn	H ₂ N—CH—COOH CH ₂ -C—NH ₂ O	5.4
aspartic acid	Asp	H ₂ N—CH—COOH CH ₂ -COOH	2.8
cysteine	Cys	H ₂ N-CH-COOH CH ₂ -SH	5.1
glutamic acid	Glu	H ₂ N-CH-COOH CH ₂ -CH ₂ -COOH	3.2
glutamine	Gln	H ₂ N-CH-COOH CH ₂ -CH ₂ -C-NH ₂ O	5.7
glycine	Gly	H ₂ N-CH ₂ -COOH	6.0
histidine	His	H ₂ N-CH-COOH CH ₂ N-N-N-N-H	7.6
isoleucine	Ile	H ₂ N-CH-COOH H ₃ C-CH-CH ₂ -CH ₃	6.0
leucine	Leu	H ₂ N-CH-COOH CH ₂ H ₃ C-CH-CH ₃	6.0

Common name	Symbol	Structural formula	pH of isoelectric point
lysine	Lys	H ₂ N-CH-COOH CH ₂ -CH ₂ -CH ₂ -CH ₂ -NH ₂	9.7
methionine	Met	H ₂ N-CH-COOH CH ₂ -CH ₂ -S-CH ₃	5.7
phenylalanine	Phe	H ₂ N-CH-COOH CH ₂	5.5
proline	Pro	COOH	6.3
serine	Ser	H ₂ N-CH-COOH CH ₂ -OH	5.7
threonine	Thr	H ₂ N-CH-COOH H ₃ C-CH-OH	5.6
tryptophan	Trp	H ₂ N-CH-COOH CH ₂	5.9
tyrosine	Tyr	H ₂ N-CH-COOH CH ₂ OH	5.7
valine	Val	H ₂ N−CH−COOH H ₃ C−CH−CH ₃	6.0

34. Lipids, carbohydrates and nucleotide components

Lipids

Octanoic acid $CH_3(CH_2)_6COOH$

Lauric acid $CH_3(CH_2)_{10}COOH$

Palmitic acid $CH_3(CH_2)_{14}COOH$

Stearic acid $CH_3(CH_2)_{16}COOH$

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

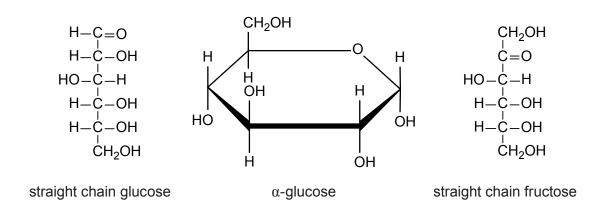
Linoleic acid $CH_3(CH_2)_4(CH=CHCH_2)_2(CH_2)_6COOH$

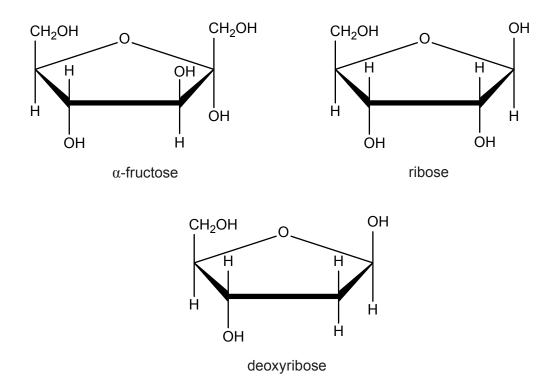
 $\alpha\text{-Linolenic acid} \qquad \text{CH}_{3}\text{CH}_{2}(\text{CH=CHCH}_{2})_{3}(\text{CH}_{2})_{6}\text{COOH}$

$$\begin{array}{c} \text{H}_{3}\text{C} \quad \text{CH}_{2} \quad \text{CH}_{2} \quad \text{CH}_{2} \\ \text{CH}_{3} \quad \text{CH}_{3} \\ \text{CH}_{3} \end{array}$$

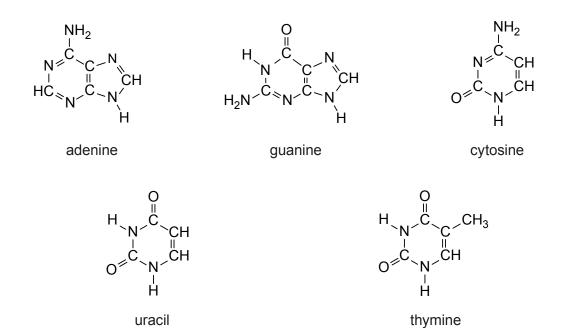
cholesterol

Carbohydrates





Nitrogenous bases



35. Vitamins and pigments

Vitamins

retinol (vitamin A)

ascorbic acid (vitamin C)

$$\begin{array}{c} H_3C \\ H_3C \\ CH \\ CH_3 \\ \end{array}$$

vitamin D (D3)

Pigments

chlorophyll

OH HO
O
$$CH_2$$
 CH_2
 CH_2
 CH_2
 CH_3
 CH_2
 CH_3
 CH_2
 CH_3
 CH_3

heme B

quinoidal base (blue)

flavylium cation (red)

 α -carotene

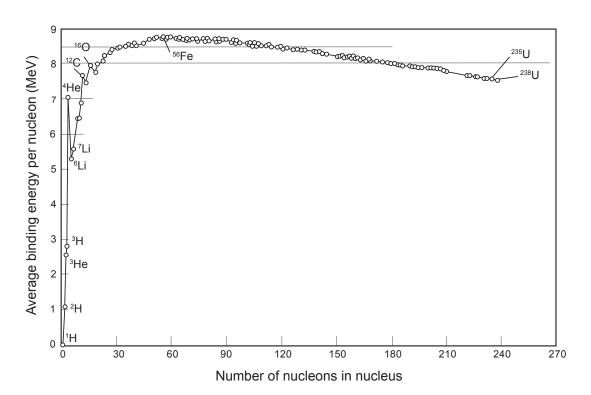
 β -carotene

Chemistry data booklet 🚯

11-cis-retinal

all-trans-retinal

36. Binding energy curve



37. Representations of some medicinal molecules

aspirin

$$H_3C$$
 CH_3 H_2C H

ibuprofen

$$H_3C-N$$
 CH_2
 CH_2
 OH
 OH

morphine

diamorphine (heroin)

penicillin (general structure)

paracetamol (acetaminophen)

$$H_3C-N$$
 CH_2
 CH_2
 CH_2
 CH_3

codeine

omeprazole

ranitidine

$$H_{3}C$$
 $H_{3}C$
 $H_{3}C$

oseltamivir

zanamivir

taxol

38. References

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

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

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

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

Data in section 13 was taken in part from:

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

Data in sections 7, 8, 9, 12, 13, 18, 19, 21, 23, 24, 28, 32 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.

