Data Booklet

for

Chemistry (Advanced Level)

for use in all papers for the H1, H2, H3 Chemistry syllabuses

TABLES OF CHEMICAL DATA

Important values, constants and standards

molar gas constant	R	$= 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$
the Faraday constant	F	$= 9.65 \times 10^4 \text{ C mol}^{-1}$
the Avogadro constant	L	$= 6.02 \times 10^{23} \text{ mol}^{-1}$
the Planck constant	h	$= 6.63 \times 10^{-34} \text{ J s}$
speed of light in a vacuum	С	$= 3.00 \times 10^8 \text{ m s}^{-1}$
rest mass of proton, ${}^{1}_{1}H$	m_{p}	$= 1.67 \times 10^{-27} \text{ kg}$
rest mass of neutron, ${}^1_0 n$	m_{n}	$= 1.67 \times 10^{-27} \text{ kg}$
rest mass of electron, $_{-1}^{0}e$	m_{e}	$= 9.11 \times 10^{-31} \text{ kg}$
electronic charge	е	$= -1.60 \times 10^{-19} C$
molar volume of gas		= 22.4 dm ³ mol ⁻¹ at s.t.p. = 24 dm ³ mol ⁻¹ under room conditions
(where s.t.p. is expressed as 101 kPa, approx		
ionic product of water	K_{W}	$= 1.00 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$

= $4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$ (= $4.18 \text{ J g}^{-1} \text{ K}^{-1}$)

(at 298 K [25 °C])

Ionisation energies (1st, 2nd, 3rd and 4th) of selected elements, in kJ mol⁻¹

	Proton Number	First	Second	Third	Fourth
Н	1	1310	-	-	-
He	2	2370	5250	-	-
Li	3	519	7300	11800	-
Ве	4	900	1760	14800	21000
В	5	799	2420	3660	25000
С	6	1090	2350	4610	6220
N	7	1400	2860	4590	7480
0	8	1310	3390	5320	7450
F	9	1680	3370	6040	8410
Ne	10	2080	3950	6150	9290
Na	11	494	4560	6940	9540
Mg	12	736	1450	7740	10500
Al	13	577	1820	2740	11600
Si	14	786	1580	3230	4360
Р	15	1060	1900	2920	4960
S	16	1000	2260	3390	4540
Cl	17	1260	2300	3850	5150
Ar	18	1520	2660	3950	5770
K	19	418	3070	4600	5860
Ca	20	590	1150	4940	6480
Sc	21	632	1240	2390	7110
Ti	22	661	1310	2720	4170
V	23	648	1370	2870	4600
Cr	24	653	1590	2990	4770
Mn	25	716	1510	3250	5190
Fe	26	762	1560	2960	5400
Co	27	757	1640	3230	5100
Ni	28	736	1750	3390	5400
Cu	29	745	1960	3350	5690
Zn	30	908	1730	3828	5980
Ga	31	577	1980	2960	6190
Ge	32	762	1540	3300	4390
Br	35	1140	2080	3460	4850
Sr	38	548	1060	4120	5440
Sn	50	707	1410	2940	3930
I	53	1010	1840	2040	4030
Ва	56	502	966	3390	-
Pb	82	716	1450	3080	4080

Bond energies

(a) Diatomic molecules

Bond	Energy/kJ mol ⁻¹
H—H	436
D—D	442
N≡N	994
O=O	496
F—F	158
C <i>l</i> —C <i>l</i>	244
Br—Br	193
I—I	151
H—F	562
H—C1	431
H—Br	366
H—I	299

(b) Polyatomic molecules

Bond	Energy/kJ mol ⁻¹
C—C	350
C=C	610
C≡C	840
C····C (benzene)	520
C—H	410
C—C1	340
C—Br	280
C—I	240
C—O	360
C=O	740
C—N	305
C=N	610
C≡N	890
N—H	390
N—N	160
N=N	410
O—H	460
0—0	150
Si—C <i>l</i>	359
Si—H	320
Si—O	444
Si—Si	222
S— C1	250
S—H	347
S—S	264

Standard electrode potential and redox potentials, E^{\ominus} at 298 K (25 °C) For ease of reference, two tabulations are given:

- (a) an extended list in alphabetical order;(b) a shorter list in decreasing order of magnitude, i.e. a redox series.

E^{\ominus} in alphabetical order (a)

Electrode re	action		$E^{\ominus}N$
$Ag^{+} + e^{-}$	=	Ag	+0.80
Al ³⁺ + 3e ⁻	=	Al	-1.66
Ba ²⁺ + 2e ⁻	=	Ва	-2.90
Br ₂ + 2e ⁻	\rightleftharpoons	2Br ⁻	+1.07
Ca ²⁺ + 2e ⁻	=	Ca	-2.87
$Cl_2 + 2e^-$	=	2C1 ⁻	+1.36
2HOC <i>l</i> + 2H ⁺ + 2e ⁻	=	$Cl_2 + 2H_2O$	+1.64
Co ²⁺ + 2e ⁻	=	Co	-0.28
Co ³⁺ + e ⁻	=	Co ²⁺	+1.82
$[Co(NH_3)_6]^{2+} + 2e^-$	=	Co + 6NH ₃	-0.43
Cr ²⁺ + 2e ⁻	=	Cr	-0.91
Cr ³⁺ + 3e ⁻	=	Cr	-0.74
Cr ³⁺ + e ⁻	=	Cr ²⁺	-0.41
$Cr_2O_7^{2-} + 14H^+ + 6e^-$	=	2Cr ³⁺ + 7H ₂ O	+1.33
Cu ⁺ + e ⁻	=	Cu	+0.52
Cu ²⁺ + 2e ⁻	=	Cu	+0.34
Cu ²⁺ + e ⁻	=	Cu⁺	+0.15
$[Cu(NH_3)_4]^{2+} + 2e^-$	=	Cu + 4NH ₃	-0.05
F ₂ + 2e ⁻	=	2F ⁻	+2.87
Fe ²⁺ + 2e ⁻	=	Fe	-0.44
Fe ³⁺ + 3e ⁻	=	Fe	-0.04
Fe ³⁺ + e ⁻	=	Fe ²⁺	+0.77
$[Fe(CN)_6]^{3-} + e^-$	=	$[Fe(CN)_6]^{4-}$	+0.36
$Fe(OH)_3 + e^-$	\rightleftharpoons	Fe(OH) ₂ + OH ⁻	-0.56
2H ⁺ + 2e ⁻	=	H_2	0.00
$I_2 + 2e^-$	=	2I ⁻	+0.54
$K^{+} + e^{-}$		K	-2.92
Li ⁺ + e [−]		Li	-3.04
Mg ²⁺ + 2e ⁻		Mg	-2.38
Mn ²⁺ + 2e ⁻		Mn	-1.18
Mn ³⁺ + e ⁻	=	Mn ²⁺	+1.49
$MnO_2 + 4H^+ + 2e^-$	=	$Mn^{2+} + 2H_2O$	+1.23
MnO ₄ + e		MnO ₄ ²⁻	+0.56
$MnO_4^- + 4H^+ + 3e^-$	=	$MnO_2 + 2H_2O$	+1.67
MnO ₄ ⁻ + 8H ⁺ + 5e ⁻	=	$Mn^{2+} + 4H_2O$	+1.52
$NO_3^- + 2H^+ + e^-$	\rightleftharpoons	$NO_2 + H_2O$	+0.81

$NO_3^- + 3H^+ + 2e^-$	=	$HNO_2 + H_2O$	+0.94
$NO_3^- + 10H^+ + 8e^-$	=	$NH_4^+ + 3H_2O$	+0.87
Na ⁺ + e ⁻	=	Na	-2.71
Ni ²⁺ + 2e ⁻	=	Ni	-0.25
$[Ni(NH_3)_6]^{2+} + 2e^-$	=	Ni + 6NH ₃	-0.51
$H_2O_2 + 2H^+ + 2e^-$	=	2H ₂ O	+1.77
$O_2 + 4H^+ + 4e^-$	\rightleftharpoons	2H ₂ O	+1.23
$O_2 + 2H_2O + 4e^-$	\rightleftharpoons	40H ⁻	+0.40
$O_2 + 2H^+ + 2e^-$	\rightleftharpoons	H_2O_2	+0.68
2H ₂ O + 2e ⁻	=	$H_2 + 2OH^-$	-0.83
Pb ²⁺ + 2e ⁻	=	Pb	-0.13
Pb ⁴⁺ + 2e ⁻	\rightleftharpoons	Pb ²⁺	+1.69
PbO ₂ + 4H ⁺ + 2e ⁻	\rightleftharpoons	$Pb^{2+} + 2H_2O$	+1.47
SO ₄ ²⁻ + 4H ⁺ + 2e ⁻	=	$SO_2 + 2H_2O$	+0.17
S ₂ O ₈ ²⁻ + 2e ⁻	\rightleftharpoons	2SO ₄ ²⁻	+2.01
S ₄ O ₆ ²⁻ + 2e ⁻	\rightleftharpoons	2S ₂ O ₃ ²⁻	+0.09
Sn ²⁺ + 2e ⁻	=	Sn	-0.14
Sn ⁴⁺ + 2e ⁻	\rightleftharpoons	Sn ²⁺	+0.15
V ²⁺ + 2e ⁻	\rightleftharpoons	V	-1.20
$V^{3+} + e^{-}$	\rightleftharpoons	V ²⁺	-0.26
VO ²⁺ + 2H ⁺ + e ⁻	=	$V^{3+} + H_2O$	+0.34
$VO_2^+ + 2H^+ + e^-$	\rightleftharpoons	$VO^{2+} + H_2O$	+1.00
$VO_3^- + 4H^+ + e^-$	=	$VO^{2+} + 2H_2O$	+1.00
Zn ²⁺ + 2e ⁻	=	Zn	-0.76

All ionic states refer to aqueous ions but other state symbols have been omitted.

(b) \mathbf{E}^{\ominus} in decreasing order of oxidising power

(see also the extended alphabetical list on the previous pages)

Electrode re		E^{\ominus}/V	
F ₂ + 2e ⁻	=	2F ⁻	+2.87
S ₂ O ₈ ²⁻ + 2e ⁻	=	2SO ₄ ²⁻	+2.01
$H_2O_2 + 2H^+ + 2e^-$	=	2H ₂ O	+1.77
$MnO_4^- + 8H^+ + 5e^-$	=	$Mn^{2+} + 4H_2O$	+1.52
$PbO_2 + 4H^+ + 2e^-$	\rightleftharpoons	$Pb^{2+} + 2H_2O$	+1.47
$Cl_2 + 2e^-$	\rightleftharpoons	2C <i>l</i> ⁻	+1.36
$Cr_2O_7^{2-} + 14H^+ + 6e^-$	=	2Cr ³⁺ + 7H ₂ O	+1.33
Br ₂ + 2e ⁻	\rightleftharpoons	2Br ⁻	+1.07
$NO_3^- + 2H^+ + e^-$	=	$NO_2 + H_2O$	+0.81
$Ag^+ + e^-$	\rightleftharpoons	Ag	+0.80
Fe ³⁺ + e ⁻	=	Fe ²⁺	+0.77
I ₂ + 2e ⁻	=	2I ⁻	+0.54
$O_2 + 2H_2O + 4e^-$	=	40H⁻	+0.40
Cu ²⁺ + 2e ⁻	=	Cu	+0.34
$SO_4^{2-} + 4H^+ + 2e^-$	=	$SO_2 + 2H_2O$	+0.17
Sn ⁴⁺ + 2e ⁻	=	Sn ²⁺	+0.15
S ₄ O ₆ ²⁻ + 2e ⁻	\rightleftharpoons	2S ₂ O ₃ ²⁻	+0.09
2H ⁺ + 2e ⁻	\rightleftharpoons	H_2	0.00
Pb ²⁺ + 2e ⁻	\rightleftharpoons	Pb	-0.13
Sn ²⁺ + 2e ⁻	\rightleftharpoons	Sn	-0.14
Fe ²⁺ + 2e ⁻	\rightleftharpoons	Fe	-0.44
Zn ²⁺ + 2e ⁻	=	Zn	-0.76
$Mg^{2+} + 2e^{-}$	=	Mg	-2.38
Ca ²⁺ + 2e ⁻	=	Ca	-2.87
K ⁺ + e ⁻	=	K	-2.92

Atomic and ionic radii

(a)	Period 3	atom	ic/nm	ionic/nm				
	metallic	Na	0.186	Na ⁺	0.095			
		Mg	0.160	Mg ²⁺	0.065			
		Al	0.143	$Aec{t}^{3+}$	0.050			
		0.	0.447	Si ⁴⁺	0.044			
	single covalent	Si	0.117	SI.	0.041			
		Р	0.110	P ³⁻	0.212			
		S	0.104	S ²⁻	0.184			
		C1	0.099	Cl ⁻	0.181			
	van der Waals	Ar	0.192					
(b)	Group II							
` '	metallic .	Be	0.112	Be ²⁺	0.031			
		Mg	0.160	Mq^{2+}	0.065			
		Ca	0.197	Mg ²⁺ Ca ²⁺ Sr ²⁺	0.099			
		Sr	0.215	Sr ²⁺	0.113			
		Ва	0.217	Ba ²⁺	0.135			
		Ra	0.220	Ra ²⁺	0.140			
(c)	Group IV							
	single covalent	С	0.077	4.				
		Si	0.117	Si ⁴⁺	0.041			
		Ge	0.122	Ge ²⁺	0.093			
	metallic	Sn	0.162	Sn ²⁺	0.112			
		Pb	0.175	Pb ²⁺	0.120			
(4)	Group VII							
(d)	single covalent	F	0.072	F ⁻	0.136			
	single covalent	C <i>l</i>	0.099	Cl ⁻	0.130			
		Br	0.114	o₁ Br¯	0.101			
		I	0.133	I_	0.193			
		At		1	0.210			
		Αι	0.140					
(e)	First row transition elemen			0.				
	single covalent	Sc	0.144	Sc ³⁺	0.081			
		Ti	0.132	Ti ²⁺	0.090			
		V	0.122	V ³⁺	0.074			
		Cr	0.117	Cr ³⁺	0.069			
		Mn	0.117	Mn ²⁺	0.080			
		Fe	0.116	Fe ²⁺	0.076			
				Fe ³⁺	0.064			
		Co	0.116	Co ²⁺	0.078			
		Ni	0.115	Ni ²⁺	0.078			
		Cu	0.117	Cu ²⁺	0.069			
		Zn	0.125	Zn^{2+}	0.074			

Characteristic values for infra-red absorption (due to stretching vibrations in organic molecules).

Bond		Characteristic ranges Wavenumber (reciprocal wavelength) /cm ⁻¹
C—Cl		700 to 800
C—O	alcohols, ethers, esters	1000 to 1300
C=C		1610 to 1680
C=O	aldehydes, ketones, acids, esters	1680 to 1750
C≡C		2070 to 2250
C≡N		2200 to 2280
О—Н	'hydrogen-bonded' in acids	2500 to 3300
С—Н	alkanes, alkenes, arenes	2840 to 3095
O—H	'hydrogen-bonded' in alcohols, phenols	3230 to 3550
N—H	primary amines	3350 to 3500
O—H	'free'	3580 to 3650

Typical proton chemical shift value (δ) relative to T.M.S.=0

Type of proton	Chemical shift (ppm)
R-CH ₃	0.9
R-CH ₂ -R	1.3
R ₃ CH	1.4–1.7
CH₃-C OR	2.0
R_CH ₃	2.1
CH ₃	2.3
R-C≡C-H	1.8–3.1
R-CH ₂ -Hal	3.2–3.7
R-O-CH ₃	3.3–4.0
R-O-H	0.5–6.0*
$R_2C=CH-$	4.5–6.0
—он	4.5–7.0*
—Н	6.0–9.0
R-CHOH	9.0–10.0
$R-C \bigcirc O \bigcirc O \bigcirc H$	9.0–13.0*
$R-NH_2$	1.0-5.0*
\sim NH $_2$	3.0-6.0*
R-CNH-	5.0–12.0*

^{*}Sensitive to solvent, concentration

S
Ξ
Φ
Ε
ō
Ш
Ф
the
<u></u>
₹
4
<u> </u>
횬
Table
<u>ဗ</u>
5
ŏ
Ξ
Φ
ᡅ
Φ
<u> </u>
⊢

	0	4.0	He	helium	2	20.2	Ne	neon	10	39.9	Ar	argon	18	83.8	궃	krypton	36	131	Xe	xenon	54	1	Rn	radon	86	I	Ono	ununoctium	118						
	IIA					19.0	ш	fluorine	9	35.5	Cl	chlorine	17	6.62	Br	bromine	35	127	Ι	iodine	53	I	At	astatine	85										
	IN					16.0	0	oxygen	8	32.1	တ	sulfur	16	0.67	Se	selenium	34	128	<u>е</u>	tellurium	52	ı	Ро	polonium	84	I	Uuh	ununhexium	116						
	^					14.0	z	nitrogen	7	31.0	۵	phosphorus	15	74.9	As	arsenic	33	122	Sp	antimony		509	Ξ	bismuth	83										
	ΛΙ					12.0	O	carbon	9	28.1	S	silicon	14	72.6	Ge	germanium	32	119	Sn	tin	50	207	Ъ	lead	82	I	Oug	ununquadium	411						
	Ш					10.8	В	boron	5	27.0	A_l	aluminium	13	2.69	Ga	gallium	31	115	In	indium	49	204	lΊ	thallium	81			-							
					'									65.4	Zn	zinc	30	112	පි	cadmium	48	201	원	mercury	80	I	qnn	ununbium	112						
														63.5	Cn	copper	29	108	Ag	silver	47	197	Αn	plog	79	I	Ouu	unununium	111						
Group														28.7	ïZ	nickel	28	106	Pd	palladium	46	195	7	platinum	78	I	Nun	ununnilium	110						
Gro														58.9	ပိ	cobalt	27	103	R	rhodium	45	192	Ir	iridium	77	I	₩	meitnerium	109						
		1.0	I	hydrogen	1									55.8	Fe	iron	26	101	Ru	ruthenium	44	190	SO	osmium	76	I	Hs	hassium	108						
						•								54.9	Mn	manganese	25	ı	С	technetium	43	186	Re	rhenium	75	I	Bh	bohrium	107						
												nass	Ю							52.0	ပ်	chromium	24	6'96	Mo	molybdenum	42	184	≯	tungsten	74	I	Sg	seaborgium	106
										Key	relative atomic mass	atomic symbol	name	nber					6.03	>	vanadium	23	92.9	qN	niobium	41	181	Та	tantalum	73	I	Op	dubnium	105	
						relati	atı		atomic number					47.9	i	titanium	22	91.2	Zr	zirconium	40	178	土	hafnium	72	I	꿆	rutherfordium	104						
														45.0	Sc	scandium	21	88.9	>	yttrium	39	139	Га	lanthanum	* 25	I	Ac	actinium *	*						
	=					9.0	Be	beryllium	4	24.3	Mg	magnesium	12	40.1	Ca	calcium	20	9.78	S	strontium	38	137	Ва	barium		I	Ra	radium	88						
	_					6.9	:=	lithium	3	23.0	Na	sodium	11	39.1	×	potassium	19	85.5	Rb	rubidium	37	133	S	caesium	22	I	Ē	francium	87						

	140	141	144	I	150	152	157	159		165		169	173	175
lanthanidae	S	Ą	ΡN	Pm	Sm	En	ВĠ	Р	٥	웃	ш	Т	Υb	n
*	cerium	praseodymium	raseodymium neodymium	promethium	samarium		gadolinium		Ε	holmium			ytterbium	lutetium
	58	59	60	61	62		64	65		67	68	69	70	71
	ı	ı	ı	1	I	1	ı	ı	ı	ı	1	I	ı	ı
* 000000	T	Ра	⊃	ď	Pu	Am	Cm	Ř	Ç	Es	Fm	Md	9 N	Lw
dellings	thorium	protactinium	uranium	neptunium	plutonium	americium	curium	berkelium	californium	einsteinium	fermium	mendelevium	nobelium	lawrencium
•	06	91	92	93	94	95	96	97	98	99	100	101	102	103