

Data Booklet

Cambridge International Advanced Subsidiary and Advanced Level in Chemistry (9701)

For use from 2016 in all papers for the above syllabus, except practical examinations.

CSTxxx





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1 Important values, constants and standards

molar gas constant	$R = 8.31 \mathrm{J}\mathrm{K}^{-1}\mathrm{mol}^{-1}$
the Faraday constant	$F = 9.65 \times 10^4 \mathrm{C} \mathrm{mol}^{-1}$
the Avogadro constant	$L = 6.02 \times 10^{23} \text{mol}^{-1}$
the Planck constant	$h = 6.63 \times 10^{-34} \mathrm{Js}$
speed of light in a vacuum	$c = 3.00 \times 10^8 \mathrm{m s^{-1}}$
rest mass of proton, ¹ ₁ H	$m_{\rm p} = 1.67 \times 10^{-27} \mathrm{kg}$
rest mass of neutron, ¹ ₀ n	$m_{\rm n} = 1.67 \times 10^{-27} \rm kg$
rest mass of electron, ⁰ ₋₁ e	$m_{\rm e} = 9.11 \times 10^{-31} \rm kg$
electronic charge	$e = -1.60 \times 10^{-19} \text{C}$
molar volume of gas	$V_{\rm m} = 22.4 {\rm dm^3 mol^{-1}}$ at s.t.p. $V_{\rm m} = 24.0 {\rm dm^3 mol^{-1}}$ under room conditions (where s.t.p. is expressed as 101 kPa, approximately, and 273 K [0 °C])
ionic product of water	$K_{\rm w} = 1.00 \times 10^{-14} \rm mol^2 dm^{-6}$ (at 298 K [25 °C])
specific heat capacity of water	= $4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$ (= $4.18 \text{ Jg}^{-1} \text{ K}^{-1}$)

2 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	7300 11800	
Be	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
Со	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
Br	35	1140	2080 3460		4850
Rb	37	403	4632 3900		5080
Sr	38	548	1060	4120	5440
Ag	47	731	2074	3361	_
I	53	1010	1840	2040	4030
Cs	55	376	2420	3300	_
Ва	56	502	966	3390	_

3 Bond Energies

3(a) Bond energies in diatomic molecules (these are exact values)

Homonuclear

Bond	Energy / kJ mol ⁻¹
н—н	436
D—D	442
N≡N	944
O=O	496
P≣P	485
S=S	425
F—F	158
Cl—Cl	242
Br—Br	193
I—I	151

Heteronuclear

Bond	Energy / kJ mol ⁻¹			
H—F	562			
H—C1	431			
H—Br	366			
H—I	299			
C≡O	1077			

3(b) Bond energies in polyatomic molecules (these are average values)

Homonuclear

Bond	Energy / kJ mol ⁻¹
с—с	350
C=C	610
C=C	840
C—C (benzene)	520
N—N	160
N=N	410
0—0	150
Si—Si	222
P—P	200
S—S	264

Heteronuclear

Bond	Energy / kJ mol ⁻¹
С—Н	410
C—C1	340
C—Br	280
C—I	240
C—N	305
C=N	610
C≡N	890
c_o	360
C=O	740
C=O in CO ₂	805
N—H	390
N—C1	310
0—Н	460
Si—C <i>l</i>	359
Si—H	320
Si—O (in SiO ₂ (s))	460
Si=O (in SiO ₂ (g))	640
P—H	320
P—C1	330
P—O	340
P=O	540
S—H	347
S—C1	250
S—0	360
S=0	500

4 Standard electrode potential and redox potentials, E^{\oplus} at 298 K (25 °C)

For ease of reference, two tables are given:

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

(a) \boldsymbol{E}^{\odot} in alphabetical order

Electrode reaction	า	E [↔] /V
$Ag^{+} + e^{-} \rightleftharpoons$ $Al^{3+} + 3e^{-} \rightleftharpoons$	Ag	+0.80
	Al	-1.66
Ba ²⁺ + 2e [−]	Ва	-2.90
$Br_2 + 2e^- \rightleftharpoons$	2Br ⁻	+1.07
Ca ²⁺ + 2e [−]	Ca	-2.87
Cl₂ + 2e ⁻	2C <i>l</i> ⁻	+1.36
2HOC <i>l</i> + 2H ⁺ + 2e ⁻	$Cl_2 + 2H_2O$	+1.64
$ClO^- + H_2O + 2e^- \rightleftharpoons$	C1 + 2OH	+0.89
Co ²⁺ + 2e [−]	Co	-0.28
Co ³⁺ + e [−]	Co ²⁺	+1.82
$[Co(NH_3)_6]^{2^+} + 2e^- \rightleftharpoons$	Co + 6NH ₃	-0.43
$Cr^{2^+} + 2e^- \rightleftharpoons$	Cr	-0.91
Cr ³⁺ + 3e [−]	Cr	-0.74
Cr ³⁺ + e [−]	Cr ²⁺	-0.41
$Cr_2O_7^{2-} + 14H^+ + 6e^- \rightleftharpoons$	2Cr ³⁺ + 7H₂O	+1.33
Cu ⁺ + e [−]	Cu	+0.52
$\begin{array}{ccc} & Cu^{+} + e^{-} & \rightleftharpoons \\ & Cu^{2+} + 2e^{-} & \rightleftharpoons \end{array}$	Cu	+0.34
Cu ²⁺ + e [−]	Cu⁺	+0.15
$[Cu(NH_3)_4]^{2^+} + 2e^- \implies$	Cu + 4NH ₃	-0.05
$Ba^{2^{+}} + 2e^{-} \rightleftharpoons Br_{2} + 2e^{-} \rightleftharpoons Ca^{2^{+}} + 2e^{-} \rightleftharpoons Cl_{2} + 2e^{-} \rightleftharpoons Cl_{2} + 2e^{-} \rightleftharpoons ClO^{-} + H_{2}O + 2e^{-} \rightleftharpoons ClO^{-} + H_{2}O + 2e^{-} \rightleftharpoons ClO^{-} + 2e^{-} = 2e^{-} + 2e^{-} = 2e^{-} = 2e^{-} + 2e^{-} = 2e^$	2F ⁻	+2.87
$ \begin{array}{ccc} F_2 + 2e^- & \rightleftharpoons \\ Fe^{2^+} + 2e^- & \rightleftharpoons \end{array} $	Fe	-0.44
Fe ³⁺ + 3e [−]	Fe	-0.04
Fe ³⁺ + e [−]	Fe ²⁺	+0.77
$[Fe(CN)_6]^{3-} + e^- \rightleftharpoons$	[Fe(CN) ₆] ⁴⁻	+0.36
Fe(OH) ₃ + e [−]	Fe(OH) ₂ + OH ⁻	-0.56
2H ⁺ + 2e [−]	H ₂	0.00
2H ₂ O + 2e ⁻	H ₂ + 2OH ⁻	-0.83
$I_2 + 2e^- \iff$	2I ⁻	+0.54
	K	-2.92
Li ⁺ + e [−] ←	Li	-3.04
Mg ²⁺ + 2e [−]	Mg	-2.38
$Mn^{2+} + 2e^- \rightleftharpoons$	Mn	-1.18
Mn ³⁺ + e [−]	Mn ²⁺	+1.49
$MnO_2 + 4H^+ + 2e^- \rightleftharpoons$	Mn ²⁺ + 2H ₂ O	+1.23
$MnO_4^- + e^- \implies$	MnO ₄ ²⁻	+0.56
$MnO_4^- + 4H^+ + 3e^- \rightleftharpoons$	MnO ₂ + 2H ₂ O	+1.67
$MnO_4^- + 8H^+ + 5e^- \rightleftharpoons$	$Mn^{2+} + 4H_2O$	+1.52
$NO_3^- + 2H^+ + e^- \rightleftharpoons$	NO ₂ + H ₂ O	+0.81
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	HNO ₂ + H ₂ O	+0.94
NO ₃ ⁻ + 10H ⁺ + 8e ⁻	NH ₄ ⁺ + 3H ₂ O	+0.87

Electrode r	eaction		E [⊕] /V
Na ⁺ + e ⁻	=	Na	-2.71
Ni ²⁺ + 2e ⁻	$\stackrel{\cdot}{\rightleftharpoons}$	Ni	-0.25
$[Ni(NH_3)_6]^{2+} + 2e^-$	\	Ni + 6NH ₃	-0.51
$H_2O_2 + 2H^+ + 2e^-$	\rightleftharpoons	2H ₂ O	+1.77
$HO_2^- + H_2O + 2e^-$	\rightleftharpoons	3OH⁻	+0.88
O ₂ + 4H ⁺ + 4e ⁻	= = = = = =	2H ₂ O	+1.23
O ₂ + 2H ₂ O + 4e ⁻	\rightleftharpoons	40H ⁻	+0.40
$O_2 + 2H^+ + 2e^-$	\rightleftharpoons	H_2O_2	+0.68
$O_2 + H_2O + 2e^-$	 	HO ₂ ⁻ + OH ⁻	-0.08
Pb ²⁺ + 2e ⁻	\rightleftharpoons	Pb	-0.13
Pb ⁴⁺ + 2e ⁻	\rightleftharpoons	Pb ²⁺	+1.69
PbO ₂ + 4H ⁺ + 2e ⁻	 	Pb ²⁺ + 2H ₂ O	+1.47
SO ₄ ²⁻ + 4H ⁺ + 2e ⁻	\rightleftharpoons	SO ₂ + 2H ₂ O	+0.17
S ₂ O ₈ ²⁻ + 2e ⁻	\rightleftharpoons	2SO ₄ ²⁻	+2.01
S ₄ O ₆ ²⁻ + 2e ⁻	\rightleftharpoons	$2S_2O_3^{2-}$	+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 ₂ O	+0.34
VO ₂ ⁺ + 2H ⁺ + e ⁻	\rightleftharpoons	VO ²⁺ + H ₂ O	+1.00
VO ₃ ⁻ + 4H ⁺ + e ⁻	\rightleftharpoons	VO ²⁺ + 2H ₂ O	+1.00
Zn ²⁺ + 2e ⁻	\rightleftharpoons	Zn	-0.76

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

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

(a selection only – see also the extended alphabetical list on the previous pages)

Electrode r	eaction		E [⊕] /V
F ₂ + 2e ⁻	=	2F ⁻	+2.87
S ₂ O ₈ ²⁻ + 2e ⁻	\rightleftharpoons	2SO ₄ ²⁻	+2.01
$H_2O_2 + 2H^+ + 2e^-$	\rightleftharpoons	2H ₂ O	+1.77
MnO ₄ ⁻ + 8H ⁺ + 5e ⁻	\rightleftharpoons	Mn ²⁺ + 4H ₂ O	+1.52
PbO ₂ + 4H ⁺ + 2e ⁻	\rightleftharpoons	Pb ²⁺ + 2H ₂ O	+1.47
Cl ₂ + 2e ⁻	\rightleftharpoons	2C1 ⁻	+1.36
$\text{Cr}_2\text{O}_7^{2-} + 14\text{H}^+ + 6\text{e}^-$	\rightleftharpoons	2Cr ³⁺ + 7H ₂ O	+1.33
O ₂ + 4H ⁺ + 4e ⁻	\rightleftharpoons	2H₂O	+1.23
Br ₂ + 2e ⁻	\rightleftharpoons	2Br ⁻	+1.07
C1O - + H2O + 2e	\rightleftharpoons	C <i>l</i> ⁻ + 2OH ⁻	+0.89
NO ₃ ⁻ + 10H ⁺ + 8e ⁻		$NH_4^+ + 3H_2O$	+0.87
NO ₃ ⁻ + 2H ⁺ + e ⁻	\rightleftharpoons	$NO_2 + H_2O$	+0.81
Ag ⁺ + e ⁻	\rightleftharpoons	Ag	+0.80
Fe ³⁺ + e ⁻	\rightleftharpoons	Fe ²⁺	+0.77
I ₂ + 2e ⁻	\rightleftharpoons	$2I^{-}$	+0.54
$O_2 + 2H_2O + 4e^-$ $Cu^{2^+} + 2e^-$	\rightleftharpoons	40H ⁻	+0.40
Cu ²⁺ + 2e ⁻	\rightleftharpoons	Cu	+0.34
SO ₄ ²⁻ + 4H ⁺ + 2e ⁻	\rightleftharpoons	SO ₂ + 2H ₂ O	+0.17
Sn ⁴⁺ + 2e ⁻	\rightleftharpoons	Sn ²⁺	+0.15
S ₄ O ₆ ²⁻ + 2e ⁻	\rightleftharpoons	$2S_2O_3^{2-}$	+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 ⁻	\rightleftharpoons	Zn	-0.76
2H ₂ O + 2e ⁻	\rightleftharpoons	H ₂ + 2OH ⁻	-0.83
V ²⁺ + 2e ⁻	\rightleftharpoons	V	-1.20
Mg ²⁺ + 2e ⁻	\rightleftharpoons	Mg	-2.38
Ca ²⁺ + 2e ⁻		Ca	-2.87
K ⁺ + e ⁻	\rightleftharpoons	K	-2.92

5 Atomic and ionic radii

(a)	Period 1	atomic/nm	ionic/nm
	single covalent	H 0.037	H⁻ 0.208
	van der Waals	He 0.140	
(b)	Period 2	atomic/nm	ionic/nm
	metallic	Li 0.152	Li ⁺ 0.060
		Be 0.112	Be ²⁺ 0.031
	single covalent	B 0.080	B ³⁺ 0.020
		C 0.077	C ⁴⁺ 0.015 C ⁴⁻ 0.260
		N 0.074	N ³⁻ 0.171
		O 0.073	O ²⁻ 0.140
		F 0.072	F- 0.136
	van der Waals	Ne 0.160	
(c)	Period 3	atomic/nm	ionic/nm
	metallic	Na 0.186	Na ⁺ 0.095
		Mg 0.160	Mg ²⁺ 0.065
		A <i>l</i> 0.143	Al ³⁺ 0.050
	single covalent	Si 0.117	Si ⁴⁺ 0.041
		P 0.110	P ³⁻ 0.212
		S 0.104	S ²⁻ 0.184
		C1 0.099	C <i>l</i> − 0.181
	van der Waals	Ar 0.190	
(d)	Group 2	atomic/nm	ionic/nm
	metallic	Be 0.112	Be ²⁺ 0.031
		Mg 0.160	Mg ²⁺ 0.065
		Ca 0.197	Ca ²⁺ 0.099
		Sr 0.215	Sr ²⁺ 0.113
		Ba 0.217	Ba ²⁺ 0.135
		Ra 0.220	Ra ²⁺ 0.140

(e)	Group 14	atomic/nm		ionic	/nm		
	single covalent	С	0.077	C ⁴⁺	0.015		
		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		
(f)	Group 17	atom	ic/nm	ionic	/nm		
	single covalent	F	0.072	F ⁻	0.136		
		Cl	0.099	Cl-	0.181		
		Br	0.114	Br ⁻	0.195		
		I	0.133	I ⁻	0.216		
		At	0.140				
(g)	First row transition elements	atom	ic/nm	ionic	nm		
	metallic	Sc	0.164			Sc ³⁺	0.081
		Ti	0.146	Ti ²⁺	0.090	Ti ³⁺	0.067
		V	0.135	V ²⁺	0.079	V ³⁺	0.064
		Cr	0.129	Cr ²⁺	0.073	Cr ³⁺	0.062
		Mn	0.132	Mn ²⁺	0.067	Mn ³⁺	0.062
		Fe	0.126	Fe ²⁺	0.061	Fe ³⁺	0.055
		Со	0.125	Co ²⁺	0.078	Co ²⁺	0.053
		Ni	0.124	Ni ²⁺	0.070	Ni ³⁺	0.056
		Cu	0.128	Cu ²⁺	0.073		
		Zn	0.135	Zn ²⁺	0.075		

6 Typical proton (1 H) chemical shift values (δ) relative to TMS = 0

type of proton	environment of proton	example structures	chemical shift range (δ)
	alkane	-CH ₃ , -CH ₂ -, >CH-	0.9–1.7
	alkyl next to C=O	CH ₃ -C=O, -CH ₂ -C=O, >CH-C=O	2.2–3.0
	alkyl next to aromatic ring	CH ₃ –Ar, –CH ₂ –Ar, >CH–Ar	2.3–3.0
	alkyl next to electronegative atom	CH ₃ –O, –CH ₂ –O, –CH ₂ –C <i>l</i> , >CH–Br	3.2–4.0
C–H	attached to alkyne	≡С–Н	1.8–3.1
C-H	attached to alkene	=CH ₂ , =CH–	4.5–6.0
	attached to aromatic ring	Н	6.0–9.0
	aldehyde	R—C H	9.3–10.5
	alcohol	RO-H	0.5–6.0
O-H (see note below)	phenol	ОН	4.5–7.0
	carboxylic acid	R—C O—H	9.0–13.0
N-H (see note below)	alkyl amine	R-NH-	1.0–5.0
	aryl amine	\sim NH $_2$	3.0-6.0
	amide	N—H	5.0–12.0

Note: δ values for –O-H and –N-H protons can vary depending on solvent and concentration

7 Typical carbon (13 C) chemical shift values (δ) relative to TMS = 0

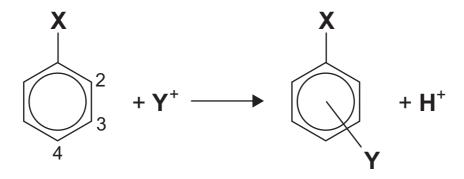
hybridisation of the carbon atom	environment of carbon atom	example structures	chemical shift range (δ)
sp ³	alkyl	CH ₃ , -CH ₂ , -CH<	0–50
sp ³	next to alkene/arene	- C H ₂ -C=C,	10–40
sp ³	next to carbonyl/carboxyl	-C H ₂ −COR, -C H ₂ −CO ₂ R	25–50
sp ³	next to nitrogen	-CH ₂ -NH ₂ , -CH ₂ -NR ₂ , -CH ₂ -NHCO	30–65
sp ³	next to chlorine (-CH ₂ -Br and -CH ₂ -I are in the same range as alkyl)	-C H ₂ −C <i>l</i>	30–60
sp ³	next to oxygen	- C H ₂ -OH, - C H ₂ -O-CO-	50–70
sp ²	alkene or arene	>C=C<, C C C	110–160
sp ²	carboxyl	R- C O ₂ H, R- C O ₂ R	160–185
sp ²	carbonyl	R-CHO, R-CO-R	190–220
sp	alkyne	R- C ≡ C -	65–85
sp nitrile		R- C ≡N	100–125

8 Characteristic infra-red absorption frequencies for some selected bonds

bond	functional groups containing the bond	absorption range (in wavenumbers) /cm ⁻¹	appearance of peak (s = strong, w = weak)
C–O	alcohols, ethers, esters	1040–1300	ø
C=C	aromatic compounds, alkenes	1500–1680	w unless conjugated
C=O	amides, ketones and aldehydes esters,	1640–1690 1670–1740 1710–1750	0 0 0
C≡C	alkynes	2150–2250	w unless conjugated
C≡N	nitriles	2200–2250	w
C–H	alkanes, CH ₂ –H alkenes/arenes, =C–H	2850–2950 3000–3100	s w
N–H	amines, amides	3300–3500	w
O–H	carboxylic acids, RCO ₂ –H H–bonded alcohol, RO–H free alcohol, RO–H	2500–3000 3200–3600 3580–3650	s and very broad s s and sharp

9 The orientating effect of groups in aromatic substitution reactions.

The position of the incoming group, \mathbf{Y} , is determined by the nature of the group, \mathbf{X} , already bonded to the ring, and not by the nature of the incoming group \mathbf{Y} .



X- groups that direct the incoming Y group to the 2- or 4- positions	X- groups that direct the incoming Y group to the 3- position	
–NH ₂ , –NHR or –NR ₂	-NO ₂	
–OH or –OR	-NH ₃	
-NHCOR	-CN	
–CH ₃ , –alkyl	-CHO, -COR	
-Cl	−CO ₂ H, −CO ₂ R	

10 Names, structures and abbreviations of some amino acids

			structure of side chain R- in
name	3-letter abbreviation	1-letter symbol	ho $ ho$
alanine	Ala	А	CH ₃ –
aspartic acid	Asp	D	HO ₂ CCH ₂ -
cysteine	Cys	С	HSCH ₂ -
glutamic acid	Glu	Е	HO ₂ CCH ₂ CH ₂ -
glycine	Gly	G	H–
lysine	Lys	К	H ₂ NCH ₂ CH ₂ CH ₂ CH ₂ -
phenylalanine	Phe	F	-CH ₂ -
serine	Ser	S	HOCH ₂ -
tyrosine	Tyr	Y	HO-CH ₂ -
valine	Val	V	CH ₃ CH-

1