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# 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.**

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## 1 Important values, constants and standards

|  |   |
|--|---|
| molar gas constant                         | $R = 8.31 \text{ JK}^{-1} \text{ mol}^{-1}$   |
| 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                        | $h = 6.63 \times 10^{-34} \text{ Js}$   |
| speed of light in a vacuum                 | $c = 3.00 \times 10^8 \text{ ms}^{-1}$  |
| rest mass of proton, ${}^1_1\text{H}$      | $m_p = 1.67 \times 10^{-27} \text{ kg}$   |
| rest mass of neutron, ${}^1_0\text{n}$     | $m_n = 1.67 \times 10^{-27} \text{ kg}$   |
| rest mass of electron, ${}^0_{-1}\text{e}$ | $m_e = 9.11 \times 10^{-31} \text{ kg}$   |
| electronic charge                          | $e = -1.60 \times 10^{-19} \text{ C}$   |
| molar volume of gas                        | $V_m = 22.4 \text{ dm}^3 \text{ mol}^{-1}$ at s.t.p.<br>$V_m = 24.0 \text{ dm}^3 \text{ mol}^{-1}$ under room conditions<br>(where s.t.p. is expressed as 101 kPa, approximately, and 273 K [0 °C]) |
| ionic product of water                     | $K_w = 1.00 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$<br>(at 298 K [25 °C])  |
| specific heat capacity of water            | $= 4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$<br>( $= 4.18 \text{ J g}^{-1} \text{ K}^{-1}$ )  |

2 Ionisation energies (1st, 2nd, 3rd and 4th) of selected elements, in  $\text{kJ mol}^{-1}$ 

|    | Proton number | First | Second | Third | Fourth |
|----|---------------|-------|--------|-------|--------|
| H  | 1             | 1310  | –      | –     | –      |
| He | 2             | 2370  | 5250   | –     | –      |
| Li | 3             | 519   | 7300   | 11800 | –      |
| Be | 4             | 900   | 1760   | 14800 | 21000  |
| B  | 5             | 799   | 2420   | 3660  | 25000  |
| C  | 6             | 1090  | 2350   | 4610  | 6220   |
| N  | 7             | 1400  | 2860   | 4590  | 7480   |
| O  | 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   |
| P  | 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   |
| 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  | –      |
| Ba | 56            | 502   | 966    | 3390  | –      |

### 3 Bond Energies

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

#### *Homonuclear*

| Bond  | Energy / $\text{kJ mol}^{-1}$ |
|-------|-------------------------------|
| H—H   | 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 / $\text{kJ mol}^{-1}$ |
|------|-------------------------------|
| H—F  | 562                           |
| H—Cl | 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 <sup>-1</sup> |
|----------------------------|-------------------------------|
| C—C                        | 350                           |
| C=C                        | 610                           |
| C≡C                        | 840                           |
| C <sup>⋯</sup> C (benzene) | 520                           |
| N—N                        | 160                           |
| N=N                        | 410                           |
| O—O                        | 150                           |
| Si—Si                      | 222                           |
| P—P                        | 200                           |
| S—S                        | 264                           |

*Heteronuclear*

| Bond                           | Energy / kJ mol <sup>-1</sup> |
|--------------------------------|-------------------------------|
| C—H                            | 410                           |
| C—Cl                           | 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 <sub>2</sub>         | 805                           |
| N—H                            | 390                           |
| N—Cl                           | 310                           |
| O—H                            | 460                           |
| Si—Cl                          | 359                           |
| Si—H                           | 320                           |
| Si—O (in SiO <sub>2</sub> (s)) | 460                           |
| Si=O (in SiO <sub>2</sub> (g)) | 640                           |
| P—H                            | 320                           |
| P—Cl                           | 330                           |
| P—O                            | 340                           |
| P=O                            | 540                           |
| S—H                            | 347                           |
| S—Cl                           | 250                           |
| S—O                            | 360                           |
| S=O                            | 500                           |

#### 4 Standard electrode potential and redox potentials, $E^\ominus$ 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) $E^\ominus$ in alphabetical order

| Electrode reaction  | $E^\ominus / V$ |
|---|-----------------|
| $Ag^+ + e^- \rightleftharpoons Ag$                                | +0.80           |
| $Al^{3+} + 3e^- \rightleftharpoons Al$                            | -1.66           |
| $Ba^{2+} + 2e^- \rightleftharpoons Ba$                            | -2.90           |
| $Br_2 + 2e^- \rightleftharpoons 2Br^-$                            | +1.07           |
| $Ca^{2+} + 2e^- \rightleftharpoons Ca$                            | -2.87           |
| $Cl_2 + 2e^- \rightleftharpoons 2Cl^-$                            | +1.36           |
| $2HOCl + 2H^+ + 2e^- \rightleftharpoons Cl_2 + 2H_2O$             | +1.64           |
| $ClO^- + H_2O + 2e^- \rightleftharpoons Cl^- + 2OH^-$             | +0.89           |
| $Co^{2+} + 2e^- \rightleftharpoons Co$                            | -0.28           |
| $Co^{3+} + e^- \rightleftharpoons Co^{2+}$                        | +1.82           |
| $[Co(NH_3)_6]^{2+} + 2e^- \rightleftharpoons Co + 6NH_3$          | -0.43           |
| $Cr^{2+} + 2e^- \rightleftharpoons Cr$                            | -0.91           |
| $Cr^{3+} + 3e^- \rightleftharpoons Cr$                            | -0.74           |
| $Cr^{3+} + e^- \rightleftharpoons Cr^{2+}$                        | -0.41           |
| $Cr_2O_7^{2-} + 14H^+ + 6e^- \rightleftharpoons 2Cr^{3+} + 7H_2O$ | +1.33           |
| $Cu^+ + e^- \rightleftharpoons Cu$                                | +0.52           |
| $Cu^{2+} + 2e^- \rightleftharpoons Cu$                            | +0.34           |
| $Cu^{2+} + e^- \rightleftharpoons Cu^+$                           | +0.15           |
| $[Cu(NH_3)_4]^{2+} + 2e^- \rightleftharpoons Cu + 4NH_3$          | -0.05           |
| $F_2 + 2e^- \rightleftharpoons 2F^-$                              | +2.87           |
| $Fe^{2+} + 2e^- \rightleftharpoons Fe$                            | -0.44           |
| $Fe^{3+} + 3e^- \rightleftharpoons Fe$                            | -0.04           |
| $Fe^{3+} + e^- \rightleftharpoons Fe^{2+}$                        | +0.77           |
| $[Fe(CN)_6]^{3-} + e^- \rightleftharpoons [Fe(CN)_6]^{4-}$        | +0.36           |
| $Fe(OH)_3 + e^- \rightleftharpoons Fe(OH)_2 + OH^-$               | -0.56           |
| $2H^+ + 2e^- \rightleftharpoons H_2$                              | 0.00            |
| $2H_2O + 2e^- \rightleftharpoons H_2 + 2OH^-$                     | -0.83           |
| $I_2 + 2e^- \rightleftharpoons 2I^-$                              | +0.54           |
| $K^+ + e^- \rightleftharpoons K$                                  | -2.92           |
| $Li^+ + e^- \rightleftharpoons Li$                                | -3.04           |
| $Mg^{2+} + 2e^- \rightleftharpoons Mg$                            | -2.38           |
| $Mn^{2+} + 2e^- \rightleftharpoons Mn$                            | -1.18           |
| $Mn^{3+} + e^- \rightleftharpoons Mn^{2+}$                        | +1.49           |
| $MnO_2 + 4H^+ + 2e^- \rightleftharpoons Mn^{2+} + 2H_2O$          | +1.23           |
| $MnO_4^- + e^- \rightleftharpoons MnO_4^{2-}$                     | +0.56           |
| $MnO_4^- + 4H^+ + 3e^- \rightleftharpoons MnO_2 + 2H_2O$          | +1.67           |
| $MnO_4^- + 8H^+ + 5e^- \rightleftharpoons Mn^{2+} + 4H_2O$        | +1.52           |
| $NO_3^- + 2H^+ + e^- \rightleftharpoons NO_2 + H_2O$              | +0.81           |
| $NO_3^- + 3H^+ + 2e^- \rightleftharpoons HNO_2 + H_2O$            | +0.94           |
| $NO_3^- + 10H^+ + 8e^- \rightleftharpoons NH_4^+ + 3H_2O$         | +0.87           |

| Electrode reaction  | $E^\ominus / V$ |
|---|-----------------|
| $\text{Na}^+ + \text{e}^- \rightleftharpoons \text{Na}$   | -2.71           |
| $\text{Ni}^{2+} + 2\text{e}^- \rightleftharpoons \text{Ni}$   | -0.25           |
| $[\text{Ni}(\text{NH}_3)_6]^{2+} + 2\text{e}^- \rightleftharpoons \text{Ni} + 6\text{NH}_3$         | -0.51           |
| $\text{H}_2\text{O}_2 + 2\text{H}^+ + 2\text{e}^- \rightleftharpoons 2\text{H}_2\text{O}$           | +1.77           |
| $\text{HO}_2^- + \text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons 3\text{OH}^-$                  | +0.88           |
| $\text{O}_2 + 4\text{H}^+ + 4\text{e}^- \rightleftharpoons 2\text{H}_2\text{O}$                     | +1.23           |
| $\text{O}_2 + 2\text{H}_2\text{O} + 4\text{e}^- \rightleftharpoons 4\text{OH}^-$                    | +0.40           |
| $\text{O}_2 + 2\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{H}_2\text{O}_2$                    | +0.68           |
| $\text{O}_2 + \text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons \text{HO}_2^- + \text{OH}^-$      | -0.08           |
| $\text{Pb}^{2+} + 2\text{e}^- \rightleftharpoons \text{Pb}$   | -0.13           |
| $\text{Pb}^{4+} + 2\text{e}^- \rightleftharpoons \text{Pb}^{2+}$                                    | +1.69           |
| $\text{PbO}_2 + 4\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{Pb}^{2+} + 2\text{H}_2\text{O}$  | +1.47           |
| $\text{SO}_4^{2-} + 4\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{SO}_2 + 2\text{H}_2\text{O}$ | +0.17           |
| $\text{S}_2\text{O}_8^{2-} + 2\text{e}^- \rightleftharpoons 2\text{SO}_4^{2-}$                      | +2.01           |
| $\text{S}_4\text{O}_6^{2-} + 2\text{e}^- \rightleftharpoons 2\text{S}_2\text{O}_3^{2-}$             | +0.09           |
| $\text{Sn}^{2+} + 2\text{e}^- \rightleftharpoons \text{Sn}$   | -0.14           |
| $\text{Sn}^{4+} + 2\text{e}^- \rightleftharpoons \text{Sn}^{2+}$                                    | +0.15           |
| $\text{V}^{2+} + 2\text{e}^- \rightleftharpoons \text{V}$   | -1.20           |
| $\text{V}^{3+} + \text{e}^- \rightleftharpoons \text{V}^{2+}$                                       | -0.26           |
| $\text{VO}^{2+} + 2\text{H}^+ + \text{e}^- \rightleftharpoons \text{V}^{3+} + \text{H}_2\text{O}$   | +0.34           |
| $\text{VO}_2^+ + 2\text{H}^+ + \text{e}^- \rightleftharpoons \text{VO}^{2+} + \text{H}_2\text{O}$   | +1.00           |
| $\text{VO}_3^- + 4\text{H}^+ + \text{e}^- \rightleftharpoons \text{VO}^{2+} + 2\text{H}_2\text{O}$  | +1.00           |
| $\text{Zn}^{2+} + 2\text{e}^- \rightleftharpoons \text{Zn}$   | -0.76           |

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



(b)  $E^\ominus$  in decreasing order of oxidising power

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

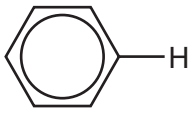
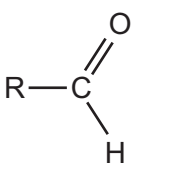
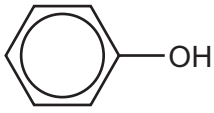
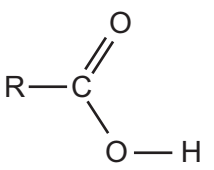
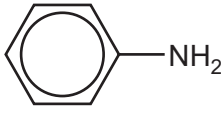
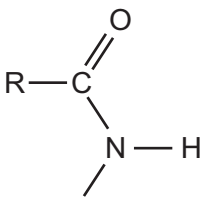
| Electrode reaction  | $E^\ominus / V$ |
|---|-----------------|
| $F_2 + 2e^- \rightleftharpoons 2F^-$                              | +2.87           |
| $S_2O_8^{2-} + 2e^- \rightleftharpoons 2SO_4^{2-}$                | +2.01           |
| $H_2O_2 + 2H^+ + 2e^- \rightleftharpoons 2H_2O$                   | +1.77           |
| $MnO_4^- + 8H^+ + 5e^- \rightleftharpoons Mn^{2+} + 4H_2O$        | +1.52           |
| $PbO_2 + 4H^+ + 2e^- \rightleftharpoons Pb^{2+} + 2H_2O$          | +1.47           |
| $Cl_2 + 2e^- \rightleftharpoons 2Cl^-$                            | +1.36           |
| $Cr_2O_7^{2-} + 14H^+ + 6e^- \rightleftharpoons 2Cr^{3+} + 7H_2O$ | +1.33           |
| $O_2 + 4H^+ + 4e^- \rightleftharpoons 2H_2O$                      | +1.23           |
| $Br_2 + 2e^- \rightleftharpoons 2Br^-$                            | +1.07           |
| $ClO^- + H_2O + 2e^- \rightleftharpoons Cl^- + 2OH^-$             | +0.89           |
| $NO_3^- + 10H^+ + 8e^- \rightleftharpoons NH_4^+ + 3H_2O$         | +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           |
| $O_2 + 2H_2O + 4e^- \rightleftharpoons 4OH^-$                     | +0.40           |
| $Cu^{2+} + 2e^- \rightleftharpoons Cu$                            | +0.34           |
| $SO_4^{2-} + 4H^+ + 2e^- \rightleftharpoons SO_2 + 2H_2O$         | +0.17           |
| $Sn^{4+} + 2e^- \rightleftharpoons Sn^{2+}$                       | +0.15           |
| $S_4O_6^{2-} + 2e^- \rightleftharpoons 2S_2O_3^{2-}$              | +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           |
| $2H_2O + 2e^- \rightleftharpoons H_2 + 2OH^-$                     | -0.83           |
| $V^{2+} + 2e^- \rightleftharpoons V$                              | -1.20           |
| $Mg^{2+} + 2e^- \rightleftharpoons Mg$                            | -2.38           |
| $Ca^{2+} + 2e^- \rightleftharpoons Ca$                            | -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 <sup>-</sup>   | 0.208 |                 |       |
| van der Waals   | He          | 0.140 |                  |       |                 |       |
| (b) Period 2    | atomic / nm |       | ionic / nm       |       |                 |       |
| metallic        | Li          | 0.152 | Li <sup>+</sup>  | 0.060 |                 |       |
|                 | Be          | 0.112 | Be <sup>2+</sup> | 0.031 |                 |       |
| single covalent | B           | 0.080 | B <sup>3+</sup>  | 0.020 |                 |       |
|                 | C           | 0.077 | C <sup>4+</sup>  | 0.015 | C <sup>4-</sup> | 0.260 |
|                 | N           | 0.074 |                  |       | N <sup>3-</sup> | 0.171 |
|                 | O           | 0.073 |                  |       | O <sup>2-</sup> | 0.140 |
|                 | F           | 0.072 |                  |       | F <sup>-</sup>  | 0.136 |
| van der Waals   | Ne          | 0.160 |                  |       |                 |       |
| (c) Period 3    | atomic / nm |       | ionic / nm       |       |                 |       |
| metallic        | Na          | 0.186 | Na <sup>+</sup>  | 0.095 |                 |       |
|                 | Mg          | 0.160 | Mg <sup>2+</sup> | 0.065 |                 |       |
|                 | Al          | 0.143 | Al <sup>3+</sup> | 0.050 |                 |       |
| single covalent | Si          | 0.117 | Si <sup>4+</sup> | 0.041 |                 |       |
|                 | P           | 0.110 |                  |       | P <sup>3-</sup> | 0.212 |
|                 | S           | 0.104 |                  |       | S <sup>2-</sup> | 0.184 |
|                 | Cl          | 0.099 |                  |       | Cl <sup>-</sup> | 0.181 |
| van der Waals   | Ar          | 0.190 |                  |       |                 |       |
| (d) Group 2     | atomic / nm |       | ionic / nm       |       |                 |       |
| metallic        | Be          | 0.112 | Be <sup>2+</sup> | 0.031 |                 |       |
|                 | Mg          | 0.160 | Mg <sup>2+</sup> | 0.065 |                 |       |
|                 | Ca          | 0.197 | Ca <sup>2+</sup> | 0.099 |                 |       |
|                 | Sr          | 0.215 | Sr <sup>2+</sup> | 0.113 |                 |       |
|                 | Ba          | 0.217 | Ba <sup>2+</sup> | 0.135 |                 |       |
|                 | Ra          | 0.220 | Ra <sup>2+</sup> | 0.140 |                 |       |

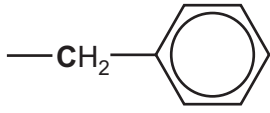
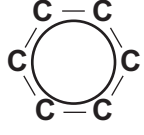
|  |                    |                        |                        |
|--|--------------------|------------------------|------------------------|
| <b>(e) Group 14</b>                      | <b>atomic / nm</b> | <b>ionic / nm</b>      |                        |
| single covalent                          | C 0.077            | C <sup>4+</sup> 0.015  |                        |
|  | Si 0.117           | Si <sup>4+</sup> 0.041 |                        |
|  | Ge 0.122           | Ge <sup>2+</sup> 0.093 |                        |
| metallic                                 | Sn 0.162           | Sn <sup>2+</sup> 0.112 |                        |
|  | Pb 0.175           | Pb <sup>2+</sup> 0.120 |                        |
| <b>(f) Group 17</b>                      | <b>atomic / nm</b> | <b>ionic / nm</b>      |                        |
| single covalent                          | F 0.072            | F <sup>-</sup> 0.136   |                        |
|  | Cl 0.099           | Cl <sup>-</sup> 0.181  |                        |
|  | Br 0.114           | Br <sup>-</sup> 0.195  |                        |
|  | I 0.133            | I <sup>-</sup> 0.216   |                        |
|  | At 0.140           |                        |                        |
| <b>(g) First row transition elements</b> | <b>atomic / nm</b> | <b>ionic / nm</b>      |                        |
| metallic                                 | Sc 0.164           |                        | Sc <sup>3+</sup> 0.081 |
|  | Ti 0.146           | Ti <sup>2+</sup> 0.090 | Ti <sup>3+</sup> 0.067 |
|  | V 0.135            | V <sup>2+</sup> 0.079  | V <sup>3+</sup> 0.064  |
|  | Cr 0.129           | Cr <sup>2+</sup> 0.073 | Cr <sup>3+</sup> 0.062 |
|  | Mn 0.132           | Mn <sup>2+</sup> 0.067 | Mn <sup>3+</sup> 0.062 |
|  | Fe 0.126           | Fe <sup>2+</sup> 0.061 | Fe <sup>3+</sup> 0.055 |
|  | Co 0.125           | Co <sup>2+</sup> 0.078 | Co <sup>2+</sup> 0.053 |
|  | Ni 0.124           | Ni <sup>2+</sup> 0.070 | Ni <sup>3+</sup> 0.056 |
|  | Cu 0.128           | Cu <sup>2+</sup> 0.073 |                        |
|  | Zn 0.135           | Zn <sup>2+</sup> 0.075 |                        |

### 6 Typical proton ( $^1\text{H}$ ) chemical shift values ( $\delta$ ) relative to TMS = 0

| type of proton          | environment of proton              | example structures  | chemical range ( $\delta$ ) |
|-------------------------|------------------------------------|---|-----------------------------|
| C-H                     | alkane                             | $-\text{CH}_3, -\text{CH}_2-, >\text{CH}-$  | 0.9–1.7                     |
|                         | alkyl next to C=O                  | $\text{CH}_3-\text{C}=\text{O}, -\text{CH}_2-\text{C}=\text{O}, >\text{CH}-\text{C}=\text{O}$ | 2.2–3.0                     |
|                         | alkyl next to aromatic ring        | $\text{CH}_3-\text{Ar}, -\text{CH}_2-\text{Ar}, >\text{CH}-\text{Ar}$                         | 2.3–3.0                     |
|                         | alkyl next to electronegative atom | $\text{CH}_3-\text{O}, -\text{CH}_2-\text{O}, -\text{CH}_2-\text{Cl}, >\text{CH}-\text{Br}$   | 3.2–4.0                     |
|                         | attached to alkyne                 | $\equiv\text{C}-\text{H}$   | 1.8–3.1                     |
|                         | attached to alkene                 | $=\text{CH}_2, =\text{CH}-$   | 4.5–6.0                     |
|                         | attached to aromatic ring          |              | 6.0–9.0                     |
|                         | aldehyde                           |             | 9.3–10.5                    |
| O-H<br>(see note below) | alcohol                            | $\text{RO}-\text{H}$  | 0.5–6.0                     |
|                         | phenol                             |            | 4.5–7.0                     |
|                         | carboxylic acid                    |            | 9.0–13.0                    |
| N-H<br>(see note below) | alkyl amine                        | $\text{R}-\text{NH}-$   | 1.0–5.0                     |
|                         | aryl amine                         |            | 3.0–6.0                     |
|                         | amide                              |            | 5.0–12.0                    |

Note:  $\delta$  values for  $-\text{O}-\text{H}$  and  $-\text{N}-\text{H}$  protons can vary depending on solvent and concentration

### 7 Typical carbon (<sup>13</sup>C) chemical shift values (δ) relative to TMS = 0

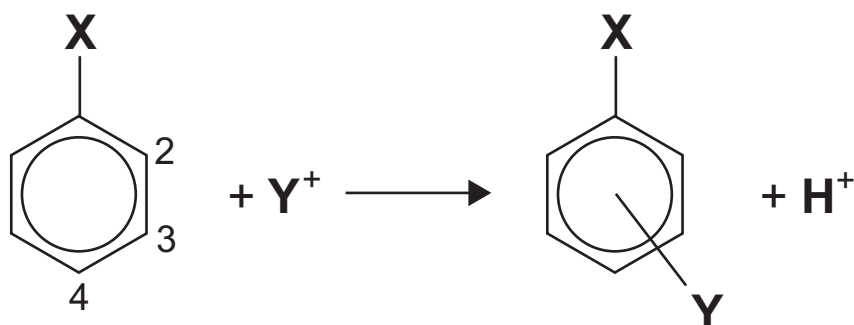
| hybridisation of the carbon atom | environment of carbon atom  | example structures  | chemical shift range (δ) |
|----------------------------------|---|---|--------------------------|
| sp <sup>3</sup>                  | alkyl   | CH <sub>3</sub> –, –CH <sub>2</sub> –, –CH<   | 0–50                     |
| sp <sup>3</sup>                  | next to alkene/arene  | –CH <sub>2</sub> –C=C,  | 10–40                    |
| sp <sup>3</sup>                  | next to carbonyl/carboxyl   | –CH <sub>2</sub> –COR, –CH <sub>2</sub> –CO <sub>2</sub> R  | 25–50                    |
| sp <sup>3</sup>                  | next to nitrogen  | –CH <sub>2</sub> –NH <sub>2</sub> , –CH <sub>2</sub> –NR <sub>2</sub> ,<br>–CH <sub>2</sub> –NHCO         | 30–65                    |
| sp <sup>3</sup>                  | next to chlorine<br>(–CH <sub>2</sub> –Br and –CH <sub>2</sub> –I are in the same range as alkyl) | –CH <sub>2</sub> –Cl  | 30–60                    |
| sp <sup>3</sup>                  | next to oxygen  | –CH <sub>2</sub> –OH, –CH <sub>2</sub> –O–CO–   | 50–70                    |
| sp <sup>2</sup>                  | alkene or arene   | >C=C<,                 | 110–160                  |
| sp <sup>2</sup>                  | carboxyl  | R–CO <sub>2</sub> H, R–CO <sub>2</sub> R  | 160–185                  |
| sp <sup>2</sup>                  | 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 <sup>-1</sup> | appearance of peak (s = strong, w = weak)                 |
|------|---|---|---|
| C–O  | alcohols, ethers, esters  | 1040–1300   | <b>s</b>  |
| C=C  | aromatic compounds, alkenes   | 1500–1680   | <b>w</b> unless conjugated                                |
| C=O  | amides, ketones and aldehydes, esters,  | 1640–1690<br>1670–1740<br>1710–1750                 | <b>s</b><br><b>s</b><br><b>s</b>                          |
| C≡C  | alkynes   | 2150–2250   | <b>w</b> unless conjugated                                |
| C≡N  | nitriles  | 2200–2250   | <b>w</b>  |
| C–H  | alkanes, CH <sub>2</sub> –H<br>alkenes/arenes, =C–H                                   | 2850–2950<br>3000–3100                              | <b>s</b><br><b>w</b>                                      |
| N–H  | amines, amides  | 3300–3500   | <b>w</b>  |
| O–H  | carboxylic acids, RCO <sub>2</sub> –H<br>H-bonded alcohol, RO–H<br>free alcohol, RO–H | 2500–3000<br>3200–3600<br>3580–3650                 | <b>s</b> and very broad<br><b>s</b><br><b>s</b> and sharp |

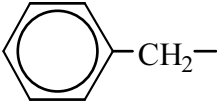
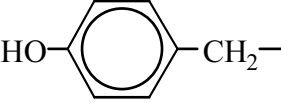
### 9 The orientating effect of groups in aromatic substitution reactions.

The position of the incoming group, **Y**, is determined by the nature of the group, **X**, already attached to the ring, and not by the nature of the incoming group **Y**.



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

### 10 Names, structures and abbreviations of some amino acids

| name          | 3-letter abbreviation | 1-letter symbol | structure of side chain R- in   |
|---------------|-----------------------|-----------------|---|
|               |                       |                 | $  \begin{array}{c}  \text{NH}_2 \\    \\  \text{R}-\text{CH} \\    \\  \text{CO}_2\text{H}  \end{array}  $ |
| alanine       | Ala                   | A               | CH <sub>3</sub> -   |
| aspartic acid | Asp                   | D               | HO <sub>2</sub> CCH <sub>2</sub> -  |
| cysteine      | Cys                   | C               | HSCH <sub>2</sub> -   |
| glutamic acid | Glu                   | E               | HO <sub>2</sub> CCH <sub>2</sub> CH <sub>2</sub> -  |
| glycine       | Gly                   | G               | H-  |
| lysine        | Lys                   | K               | H <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> -                           |
| phenylalanine | Phe                   | F               |                          |
| serine        | Ser                   | S               | HOCH <sub>2</sub> -   |
| tyrosine      | Tyr                   | Y               |                         |
| valine        | Val                   | V               | $  \begin{array}{c}  \text{CH}_3 \\    \\  \text{CH}- \\    \\  \text{CH}_3  \end{array}  $                 |



# The Periodic Table of Elements

| Group                               |                                      |  |  |                                      |                                       |                                      |                                       |                                     |                                       |                                      |                                      |                                      |                                      |                                      |                                       |                                     |                                    |  |  |  |  |
|-------------------------------------|--------------------------------------|--|--|--------------------------------------|---------------------------------------|--------------------------------------|---------------------------------------|-------------------------------------|---------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|---------------------------------------|-------------------------------------|------------------------------------|--|--|--|--|
| 1                                   | 2                                    |  |  |                                      |                                       |                                      |                                       |                                     |                                       |                                      |                                      | 13                                   | 14                                   | 15                                   | 16                                    | 17                                  | 18                                 |  |  |  |  |
|                                     |                                      | <b>Key</b>   |  |                                      |                                       |                                      |                                       |                                     |                                       |                                      |                                      |                                      |                                      |                                      |                                       |                                     |                                    |  |  |  |  |
|                                     |                                      | atomic number<br>atomic symbol<br>name<br>relative atomic mass |  |                                      |                                       |                                      |                                       |                                     |                                       |                                      |                                      | 1<br>H<br>hydrogen<br>1.0            |                                      |                                      |                                       |                                     |                                    |  |  |  |  |
| 3<br><b>Li</b><br>lithium<br>6.9    | 4<br><b>Be</b><br>beryllium<br>9.0   |  |  |                                      |                                       |                                      |                                       |                                     |                                       |                                      |                                      | 5<br><b>B</b><br>boron<br>10.8       | 6<br><b>C</b><br>carbon<br>12.0      | 7<br><b>N</b><br>nitrogen<br>14.0    | 8<br><b>O</b><br>oxygen<br>16.0       | 9<br><b>F</b><br>fluorine<br>19.0   | 10<br><b>Ne</b><br>neon<br>20.2    |  |  |  |  |
| 11<br><b>Na</b><br>sodium<br>23.0   | 12<br><b>Mg</b><br>magnesium<br>24.3 | 3  | 4                                      | 5                                    | 6                                     | 7                                    | 8                                     | 9                                   | 10                                    | 11                                   | 12                                   | 13<br><b>Al</b><br>aluminium<br>27.0 | 14<br><b>Si</b><br>silicon<br>28.1   | 15<br><b>P</b><br>phosphorus<br>31.0 | 16<br><b>S</b><br>sulfur<br>32.1      | 17<br><b>Cl</b><br>chlorine<br>35.5 | 18<br><b>Ar</b><br>argon<br>39.9   |  |  |  |  |
| 19<br><b>K</b><br>potassium<br>39.1 | 20<br><b>Ca</b><br>calcium<br>40.1   | 21<br><b>Sc</b><br>scandium<br>45.0                            | 22<br><b>Ti</b><br>titanium<br>47.9    | 23<br><b>V</b><br>vanadium<br>50.9   | 24<br><b>Cr</b><br>chromium<br>52.0   | 25<br><b>Mn</b><br>manganese<br>54.9 | 26<br><b>Fe</b><br>iron<br>55.8       | 27<br><b>Co</b><br>cobalt<br>58.9   | 28<br><b>Ni</b><br>nickel<br>58.7     | 29<br><b>Cu</b><br>copper<br>63.5    | 30<br><b>Zn</b><br>zinc<br>65.4      | 31<br><b>Ga</b><br>gallium<br>69.7   | 32<br><b>Ge</b><br>germanium<br>72.6 | 33<br><b>As</b><br>arsenic<br>74.9   | 34<br><b>Se</b><br>selenium<br>79.0   | 35<br><b>Br</b><br>bromine<br>79.9  | 36<br><b>Kr</b><br>krypton<br>83.8 |  |  |  |  |
| 37<br><b>Rb</b><br>rubidium<br>85.5 | 38<br><b>Sr</b><br>strontium<br>87.6 | 39<br><b>Y</b><br>yttrium<br>88.9                              | 40<br><b>Zr</b><br>zirconium<br>91.2   | 41<br><b>Nb</b><br>niobium<br>92.9   | 42<br><b>Mo</b><br>molybdenum<br>95.9 | 43<br><b>Tc</b><br>technetium<br>–   | 44<br><b>Ru</b><br>ruthenium<br>101.1 | 45<br><b>Rh</b><br>rhodium<br>102.9 | 46<br><b>Pd</b><br>palladium<br>106.4 | 47<br><b>Ag</b><br>silver<br>107.9   | 48<br><b>Cd</b><br>cadmium<br>112.4  | 49<br><b>In</b><br>indium<br>114.8   | 50<br><b>Sn</b><br>tin<br>116.7      | 51<br><b>Sb</b><br>antimony<br>121.8 | 52<br><b>Te</b><br>tellurium<br>127.6 | 53<br><b>I</b><br>iodine<br>126.9   | 54<br><b>Xe</b><br>xenon<br>131.3  |  |  |  |  |
| 55<br><b>Cs</b><br>caesium<br>132.9 | 56<br><b>Ba</b><br>barium<br>137.3   | 57–71<br>lanthanoids   | 72<br><b>Hf</b><br>hafnium<br>178.5    | 73<br><b>Ta</b><br>tantalum<br>180.9 | 74<br><b>W</b><br>tungsten<br>183.8   | 75<br><b>Re</b><br>rhenium<br>186.2  | 76<br><b>Os</b><br>osmium<br>190.2    | 77<br><b>Ir</b><br>iridium<br>192.2 | 78<br><b>Pt</b><br>platinum<br>195.1  | 79<br><b>Au</b><br>gold<br>197.0     | 80<br><b>Hg</b><br>mercury<br>200.6  | 81<br><b>Tl</b><br>thallium<br>204.4 | 82<br><b>Pb</b><br>lead<br>207.2     | 83<br><b>Bi</b><br>bismuth<br>209.0  | 84<br><b>Po</b><br>polonium<br>–      | 85<br><b>At</b><br>astatine<br>–    | 86<br><b>Rn</b><br>radon<br>–      |  |  |  |  |
| 87<br><b>Fr</b><br>francium<br>–    | 88<br><b>Ra</b><br>radium<br>–       | 89–103<br>actinoids  | 104<br><b>Rf</b><br>rutherfordium<br>– | 105<br><b>Db</b><br>dubnium<br>–     | 106<br><b>Sg</b><br>seaborgium<br>–   | 107<br><b>Bh</b><br>bohrium<br>–     | 108<br><b>Hs</b><br>hassium<br>–      | 109<br><b>Mt</b><br>meitnerium<br>– | 110<br><b>Ds</b><br>darmstadtium<br>– | 111<br><b>Rg</b><br>roentgenium<br>– | 112<br><b>Cn</b><br>copernicium<br>– |                                      | 114<br><b>Fl</b><br>flerovium<br>–   |                                      | 116<br><b>Lv</b><br>livermorium<br>–  |                                     |                                    |  |  |  |  |

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|             |                                       |                                    |  |                                       |                                    |                                      |                                      |  |                                     |  |                                     |                                    |                                     |                                       |                                      |
|-------------|---------------------------------------|------------------------------------|--|---------------------------------------|------------------------------------|--------------------------------------|--------------------------------------|--|-------------------------------------|--|-------------------------------------|------------------------------------|-------------------------------------|---------------------------------------|--------------------------------------|
| lanthanoids | 57<br><b>La</b><br>lanthanum<br>138.9 | 58<br><b>Ce</b><br>cerium<br>140.1 | 59<br><b>Pr</b><br>praseodymium<br>140.9 | 60<br><b>Nd</b><br>neodymium<br>144.4 | 61<br><b>Pm</b><br>promethium<br>– | 62<br><b>Sm</b><br>samarium<br>150.4 | 63<br><b>Eu</b><br>europium<br>152.0 | 64<br><b>Gd</b><br>gadolinium<br>157.3 | 65<br><b>Tb</b><br>terbium<br>158.9 | 66<br><b>Dy</b><br>dysprosium<br>162.5 | 67<br><b>Ho</b><br>holmium<br>164.9 | 68<br><b>Er</b><br>erbium<br>167.3 | 69<br><b>Tm</b><br>thulium<br>168.9 | 70<br><b>Yb</b><br>ytterbium<br>173.1 | 71<br><b>Lu</b><br>lutetium<br>175.0 |
| actinoids   | 89<br><b>Ac</b><br>actinium           | 90<br><b>Th</b><br>thorium         | 91<br><b>Pa</b><br>protactinium          | 92<br><b>U</b><br>uranium             | 93<br><b>Np</b><br>neptunium       | 94<br><b>Pu</b><br>plutonium         | 95<br><b>Am</b><br>americium         | 96<br><b>Cm</b><br>curium              | 97<br><b>Bk</b><br>berkelium        | 98<br><b>Cf</b><br>californium         | 99<br><b>Es</b><br>einsteinium      | 100<br><b>Fm</b><br>fermium        | 101<br><b>Md</b><br>mendelevium     | 102<br><b>No</b><br>nobelium          | 103<br><b>Lr</b><br>lawrencium<br>–  |

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