

Cambridge
International
AS & A Level

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 | $R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$ |
| 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 | $c = 3.00 \times 10^8 \text{ m s}^{-1}$ |
| 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. $V_m = 24.0 \text{ dm}^3 \text{ mol}^{-1}$ under room conditions (where s.t.p. is expressed as 101 kPa, approximately, and 273 K [0 °C]) |
| ionic product of water | $K_w = 1.00 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$ (at 298 K [25 °C]) |
| specific heat capacity of water | $= 4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$ (= $4.18 \text{ J g}^{-1} \text{ K}^{-1}$) |

2 Ionisation energies (1st, 2nd, 3rd and 4th) of selected elements, in kJmol^{-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 / kJ mol^{-1} |
|--------------------------|-------------------------------|
| H H | 436 |
| D D | 442 |
| $\text{N}\equiv\text{N}$ | 944 |
| $\text{O}=\text{O}$ | 496 |
| $\text{P}\equiv\text{P}$ | 485 |
| $\text{S}=\text{S}$ | 425 |
| F F | 158 |
| Cl Cl | 242 |
| Br Br | 193 |
| I I | 151 |

Heteronuclear

| Bond | Energy / kJ mol^{-1} |
|--------------------------|-------------------------------|
| H F | 562 |
| H Cl | 431 |
| H Br | 366 |
| H I | 299 |
| $\text{C}\equiv\text{O}$ | 1077 |

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

Homonuclear

| Bond | Energy / kJ mol ⁻¹ |
|----------------------------|-------------------------------|
| C C | 350 |
| C=C | 610 |
| C≡C | 840 |
| C [⋯] 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 ⁻¹ |
|--------------------------------|-------------------------------|
| 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 ₂ | 805 |
| N H | 390 |
| N Cl | 310 |
| O H | 460 |
| Si Cl | 359 |
| Si H | 320 |
| Si O (in SiO ₂ (s)) | 460 |
| Si=O (in SiO ₂ (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 |
|--|-----------------|
| $\text{Ag}^+ + \text{e}^- \rightleftharpoons \text{Ag}$ | +0.80 |
| $\text{Al}^{3+} + 3\text{e}^- \rightleftharpoons \text{Al}$ | -1.66 |
| $\text{Ba}^{2+} + 2\text{e}^- \rightleftharpoons \text{Ba}$ | -2.90 |
| $\text{Br}_2 + 2\text{e}^- \rightleftharpoons 2\text{Br}^-$ | +1.07 |
| $\text{Ca}^{2+} + 2\text{e}^- \rightleftharpoons \text{Ca}$ | -2.87 |
| $\text{Cl}_2 + 2\text{e}^- \rightleftharpoons 2\text{Cl}^-$ | +1.36 |
| $2\text{HOCl} + 2\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{Cl}_2 + 2\text{H}_2\text{O}$ | +1.64 |
| $\text{ClO}^- + \text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons \text{Cl}^- + 2\text{OH}^-$ | +0.89 |
| $\text{Co}^{2+} + 2\text{e}^- \rightleftharpoons \text{Co}$ | -0.28 |
| $\text{Co}^{3+} + \text{e}^- \rightleftharpoons \text{Co}^{2+}$ | +1.82 |
| $[\text{Co}(\text{NH}_3)_6]^{2+} + 2\text{e}^- \rightleftharpoons \text{Co} + 6\text{NH}_3$ | -0.43 |
| $\text{Cr}^{2+} + 2\text{e}^- \rightleftharpoons \text{Cr}$ | -0.91 |
| $\text{Cr}^{3+} + 3\text{e}^- \rightleftharpoons \text{Cr}$ | -0.74 |
| $\text{Cr}^{3+} + \text{e}^- \rightleftharpoons \text{Cr}^{2+}$ | -0.41 |
| $\text{Cr}_2\text{O}_7^{2-} + 14\text{H}^+ + 6\text{e}^- \rightleftharpoons 2\text{Cr}^{3+} + 7\text{H}_2\text{O}$ | +1.33 |
| $\text{Cu}^+ + \text{e}^- \rightleftharpoons \text{Cu}$ | +0.52 |
| $\text{Cu}^{2+} + 2\text{e}^- \rightleftharpoons \text{Cu}$ | +0.34 |
| $\text{Cu}^{2+} + \text{e}^- \rightleftharpoons \text{Cu}^+$ | +0.15 |
| $[\text{Cu}(\text{NH}_3)_4]^{2+} + 2\text{e}^- \rightleftharpoons \text{Cu} + 4\text{NH}_3$ | -0.05 |
| $\text{F}_2 + 2\text{e}^- \rightleftharpoons 2\text{F}^-$ | +2.87 |
| $\text{Fe}^{2+} + 2\text{e}^- \rightleftharpoons \text{Fe}$ | -0.44 |
| $\text{Fe}^{3+} + 3\text{e}^- \rightleftharpoons \text{Fe}$ | -0.04 |
| $\text{Fe}^{3+} + \text{e}^- \rightleftharpoons \text{Fe}^{2+}$ | +0.77 |
| $[\text{Fe}(\text{CN})_6]^{3-} + \text{e}^- \rightleftharpoons [\text{Fe}(\text{CN})_6]^{4-}$ | +0.36 |
| $\text{Fe}(\text{OH})_3 + \text{e}^- \rightleftharpoons \text{Fe}(\text{OH})_2 + \text{OH}^-$ | -0.56 |
| $2\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{H}_2$ | 0.00 |
| $2\text{H}_2\text{O} + 2\text{e}^- \rightleftharpoons \text{H}_2 + 2\text{OH}^-$ | -0.83 |
| $\text{I}_2 + 2\text{e}^- \rightleftharpoons 2\text{I}^-$ | +0.54 |
| $\text{K}^+ + \text{e}^- \rightleftharpoons \text{K}$ | -2.92 |
| $\text{Li}^+ + \text{e}^- \rightleftharpoons \text{Li}$ | -3.04 |
| $\text{Mg}^{2+} + 2\text{e}^- \rightleftharpoons \text{Mg}$ | -2.38 |
| $\text{Mn}^{2+} + 2\text{e}^- \rightleftharpoons \text{Mn}$ | -1.18 |
| $\text{Mn}^{3+} + \text{e}^- \rightleftharpoons \text{Mn}^{2+}$ | +1.49 |
| $\text{MnO}_2 + 4\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{Mn}^{2+} + 2\text{H}_2\text{O}$ | +1.23 |
| $\text{MnO}_4^- + \text{e}^- \rightleftharpoons \text{MnO}_4^{2-}$ | +0.56 |
| $\text{MnO}_4^- + 4\text{H}^+ + 3\text{e}^- \rightleftharpoons \text{MnO}_2 + 2\text{H}_2\text{O}$ | +1.67 |
| $\text{MnO}_4^- + 8\text{H}^+ + 5\text{e}^- \rightleftharpoons \text{Mn}^{2+} + 4\text{H}_2\text{O}$ | +1.52 |
| $\text{NO}_3^- + 2\text{H}^+ + \text{e}^- \rightleftharpoons \text{NO}_2 + \text{H}_2\text{O}$ | +0.81 |
| $\text{NO}_3^- + 3\text{H}^+ + 2\text{e}^- \rightleftharpoons \text{HNO}_2 + \text{H}_2\text{O}$ | +0.94 |
| $\text{NO}_3^- + 10\text{H}^+ + 8\text{e}^- \rightleftharpoons \text{NH}_4^+ + 3\text{H}_2\text{O}$ | +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)

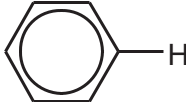
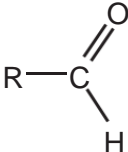
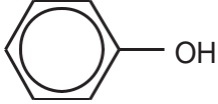
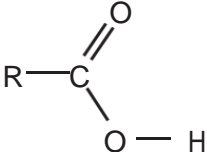
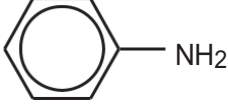
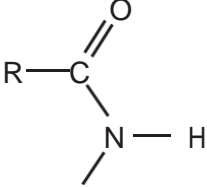
| Electrode reaction | E^\ominus / V |
|---|-----------------|
| $F_2 + 2e^- \rightleftharpoons 2F^-$ | +2.87 |
| $S_2O_8^{2-} + 2e^- \rightleftharpoons 2SO_4^{2-}$ | +2.01 |
| $H_2O_2 + 2H^+ + 2e^- \rightleftharpoons 2H_2O$ | +1.77 |
| $MnO_4^- + 8H^+ + 5e^- \rightleftharpoons Mn^{2+} + 4H_2O$ | +1.52 |
| $PbO_2 + 4H^+ + 2e^- \rightleftharpoons Pb^{2+} + 2H_2O$ | +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 ⁻ | 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 |
| | | Al 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 |
| | | Cl 0.099 | | Cl ⁻ 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 |

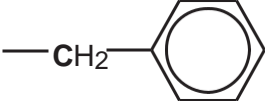
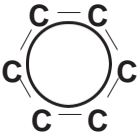
| | | | | |
|-----|-------------------------------|------------|------------------------|------------------------|
| (e) | Group 14 | atomic/ nm | ionic/ nm | |
| | single covalent | C 0.077 | C ⁴⁺ 0.015 | |
| | | Si 0.117 | Si ⁴⁺ 0.041 | |
| | | Ge 0.122 | Ge ²⁺ 0.093 | |
| | metallic | Sn 0.162 | Sn ²⁺ 0.112 | |
| | | Pb 0.175 | Pb ²⁺ 0.120 | |
| (f) | Group 17 | atomic/ 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 | atomic/ 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 |
| | | Co 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 (^1H) chemical shift values (δ) relative to TMS = 0

| type of proton | environment of proton | example structures | chemical shift range (δ) |
|-------------------------|------------------------------------|---|-----------------------------------|
| 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 (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 (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: δ values for $-\text{O}-\text{H}$ and $-\text{N}-\text{H}$ 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- , $-\text{CH}_2-$, $-\text{CH}<$ | 0–50 |
| sp^3 | next to alkene/arene | $-\text{CH}_2-\text{C}=\text{C}$,  | 10–40 |
| sp^3 | next to carbonyl/carboxyl | $-\text{CH}_2-\text{COR}$, $-\text{CH}_2-\text{CO}_2\text{R}$ | 25–50 |
| sp^3 | next to nitrogen | $-\text{CH}_2-\text{NH}_2$, $-\text{CH}_2-\text{NR}_2$, $-\text{CH}_2-\text{NHCO}$ | 30–65 |
| sp^3 | next to chlorine ($-\text{CH}_2-\text{Br}$ and $-\text{CH}_2-\text{I}$ are in the same range as alkyl) | $-\text{CH}_2-\text{Cl}$ | 30–60 |
| sp^3 | next to oxygen | $-\text{CH}_2-\text{OH}$, $-\text{CH}_2-\text{O}-\text{CO}-$ | 50–70 |
| sp^2 | alkene or arene | $>\text{C}=\text{C}<$,  | 110–160 |
| sp^2 | carboxyl | $\text{R}-\text{CO}_2\text{H}$, $\text{R}-\text{CO}_2\text{R}$ | 160–185 |
| sp^2 | carbonyl | $\text{R}-\text{CHO}$, $\text{R}-\text{CO}-\text{R}$ | 190–220 |
| sp | alkyne | $\text{R}-\text{C}\equiv\text{C}-$ | 65–85 |
| sp | nitrile | $\text{R}-\text{C}\equiv\text{N}$ | 100–125 |

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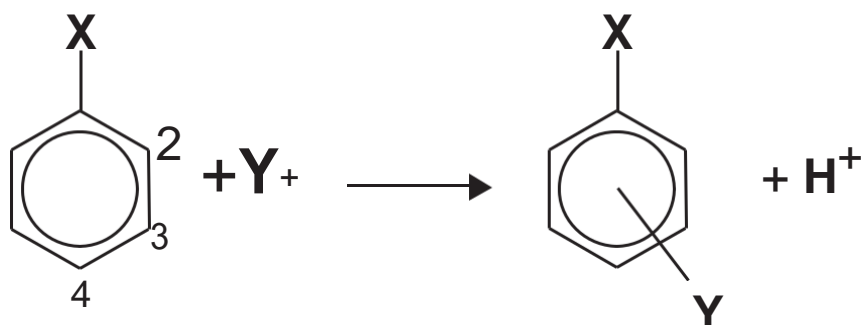
8 Characteristic infra-red absorption frequencies for some selected bonds

| 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 | s |
| C=C | aromatic compounds, alkenes | 1500–1680 | w unless conjugated |
| C=O | amides, ketones and aldehydes, esters, | 1640–1690 1670–1740 1710–1750 | s s s |
| 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 |

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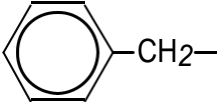
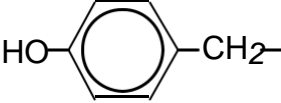
9 The orientating effect of groups in aromatic substitution reactions.

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

| 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 ₃ - |
| aspartic acid | Asp | D | HO ₂ CCH ₂ - |
| cysteine | Cys | C | HSCH ₂ - |
| glutamic acid | Glu | E | HO ₂ CCH ₂ CH ₂ - |
| glycine | Gly | G | H- |
| lysine | Lys | K | H ₂ NCH ₂ CH ₂ CH ₂ CH ₂ - |
| phenylalanine | Phe | F |  |
| serine | Ser | S | HOCH ₂ - |
| tyrosine | Tyr | Y |  |
| valine | Val | V | $\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}- \\ \\ \text{CH}_3 \end{array}$ |

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The Periodic Table of Elements

| Group | | | | | | | | | | | | | | | | | |
|------------------------------|-------------------------------|---|---------------------------------|-------------------------------|--------------------------------|-------------------------------|--------------------------------|------------------------------|--------------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|--------------------------------|------------------------------|-----------------------------|
| 1 | 2 | | | | | | | | | | | 13 | 14 | 15 | 16 | 17 | 18 |
| | | | | | | | | | | | 1 H hydrogen 1.0 | | | | | | 2 He helium 4.0 |
| 3 Li lithium 6.9 | 4 Be beryllium 9.0 | <div style="border: 1px solid black; padding: 5px; display: inline-block;"> Key atomic number atomic symbol name relative atomic mass </div> | | | | | | | | | | 5 B boron 10.8 | 6 C carbon 12.0 | 7 N nitrogen 14.0 | 8 O oxygen 16.0 | 9 F fluorine 19.0 | 10 Ne neon 20.2 |
| 11 Na sodium 23.0 | 12 Mg magnesium 24.3 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 Al aluminium 27.0 | 14 Si silicon 28.1 | 15 P phosphorus 31.0 | 16 S sulfur 32.1 | 17 Cl chlorine 35.5 | 18 Ar argon 39.9 |
| 19 K potassium 39.1 | 20 Ca calcium 40.1 | 21 Sc scandium 45.0 | 22 Ti titanium 47.9 | 23 V vanadium 50.9 | 24 Cr chromium 52.0 | 25 Mn manganese 54.9 | 26 Fe iron 55.8 | 27 Co cobalt 58.9 | 28 Ni nickel 58.7 | 29 Cu copper 63.5 | 30 Zn zinc 65.4 | 31 Ga gallium 69.7 | 32 Ge germanium 72.6 | 33 As arsenic 74.9 | 34 Se selenium 79.0 | 35 Br bromine 79.9 | 36 Kr krypton 83.8 |
| 37 Rb rubidium 85.5 | 38 Sr strontium 87.6 | 39 Y yttrium 88.9 | 40 Zr zirconium 91.2 | 41 Nb niobium 92.9 | 42 Mo molybdenum 95.9 | 43 Tc technetium - | 44 Ru ruthenium 101.1 | 45 Rh rhodium 102.9 | 46 Pd palladium 106.4 | 47 Ag silver 107.9 | 48 Cd cadmium 112.4 | 49 In indium 114.8 | 50 Sn tin 116.7 | 51 Sb antimony 121.8 | 52 Te tellurium 127.6 | 53 I iodine 126.9 | 54 Xe xenon 131.3 |
| 55 Cs caesium 132.9 | 56 Ba barium 137.3 | 57-71 lanthanoids | 72 Hf hafnium 178.5 | 73 Ta tantalum 180.9 | 74 W tungsten 183.8 | 75 Re rhenium 186.2 | 76 Os osmium 190.2 | 77 Ir iridium 192.2 | 78 Pt platinum 195.1 | 79 Au gold 197.0 | 80 Hg mercury 200.6 | 81 Tl thallium 204.4 | 82 Pb lead 207.2 | 83 Bi bismuth 209.0 | 84 Po polonium - | 85 At astatine - | 86 Rn radon - |
| 87 Fr francium - | 88 Ra radium - | 89-103 actinoids | 104 Rf rutherfordium - | 105 Db dubnium - | 106 Sg seaborgium - | 107 Bh bohrium - | 108 Hs hassium - | 109 Mt meitnerium - | 110 Ds darmstadtium - | 111 Rg roentgenium - | 112 Cr copernicium - | | 114 Fl flerovium - | | 116 Lv livermorium - | | |

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| | | | | | | | | | | | | | | | |
|-------------|--------------------------------|------------------------------|-----------------------------------|--------------------------------|-----------------------------|-------------------------------|-------------------------------|---------------------------------|------------------------------|---------------------------------|------------------------------|-----------------------------|-------------------------------|--------------------------------|-------------------------------|
| lanthanoids | 57 La lanthanum 138.9 | 58 Ce cerium 140.1 | 59 Pr praseodymium 140.9 | 60 Nd neodymium 144.4 | 61 Pm promethium - | 62 Sm samarium 150.4 | 63 Eu europium 152.0 | 64 Gd gadolinium 157.3 | 65 Tb terbium 158.9 | 66 Dy dysprosium 162.5 | 67 Ho holmium 164.9 | 68 Er erbium 167.3 | 69 Tm thulium 168.9 | 70 Yb ytterbium 173.1 | 71 Lu lutetium 175.0 |
| actinoids | 89 Ac actinium - | 90 Th thorium 232.0 | 91 Pa protactinium 231.0 | 92 U uranium 238.0 | 93 Np neptunium - | 94 Pu plutonium - | 95 Am americium - | 96 Cm curium - | 97 Bk berkelium - | 98 Cf californium - | 99 Es einsteinium - | 100 Fm fermium - | 101 Md mendelevium - | 102 No nobelium - | 103 Lr lawrencium - |