

Chemistry data booklet

For use during the course and in the examinations
First assessment 2025

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Diploma Programme

Chemistry data booklet

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Introduction

This Diploma Programme (DP) *Chemistry data booklet* accompanies the DP *Chemistry guide* and DP *Chemistry teacher support material*. It contains chemical and physical equations and constants, chemical symbols, the periodic table, and other chemical data relevant to the course.

Students must have access to a copy of this booklet for the duration of the course, so that they can become familiar with its contents. Direct reference is made to relevant equations in the “Understandings” sections of the guide. This helps to maintain the emphasis on interpretation and application rather than memorization of symbols, constants and equations.

Each student must have access to a clean copy of the *Chemistry data booklet* during examinations. It is the responsibility of the school to download a copy of this booklet from IBIS or the Programme Resource Centre and to ensure that there are sufficient copies available for all students.

1. Some relevant equations

| Equation |
|---|
| $c = f\lambda$ |
| $E = hf$ |
| $n = \frac{m}{M}$ |
| $n = CV$ |
| $PV = nRT$ |
| $\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$ |
| $Q = mc\Delta T$ |
| $\% \text{ atom economy} = \frac{\text{molar mass of desired product}}{\text{molar mass of all reactants}} \times 100$ |
| $\Delta H^\ominus = \sum(\Delta H_{\text{f}}^\ominus \text{ products}) - \sum(\Delta H_{\text{f}}^\ominus \text{ reactants})$ |
| $\Delta H^\ominus = \sum(\Delta H_{\text{c}}^\ominus \text{ reactants}) - \sum(\Delta H_{\text{c}}^\ominus \text{ products})$ |
| $\Delta G^\ominus = \Delta H^\ominus - T\Delta S^\ominus$ |
| $\Delta G = \Delta G^\ominus + RT \ln Q$ |
| $\Delta G^\ominus = -RT \ln K$ |
| $\Delta G^\ominus = -nFE^\ominus$ |
| $k = Ae^{\frac{-E_a}{RT}}$ |
| $\ln k = \frac{-E_a}{RT} + \ln A$ |
| $\text{pH} = -\log_{10} [\text{H}_3\text{O}^+]$ or $\text{pH} = -\log_{10} [\text{H}^+]$ |
| $K_w = [\text{H}^+][\text{OH}^-]$ |
| $\text{pOH} = -\log_{10} [\text{OH}^-]$ |

2. Physical constants

| Quantity | Symbol | Approximate value |
|--|--------|---|
| Elementary charge | e | $1.602177 \times 10^{-19} \text{ C}$ |
| Electron rest mass | m_e | $9.109384 \times 10^{-31} \text{ kg}$ |
| Proton rest mass | m_p | $1.672622 \times 10^{-27} \text{ kg}$ |
| Neutron rest mass | m_n | $1.674927 \times 10^{-27} \text{ kg}$ |
| Speed of light in vacuum | c | $3.00 \times 10^8 \text{ m s}^{-1}$ |
| Planck constant | h | $6.63 \times 10^{-34} \text{ J s}$ |
| Avogadro constant | N_A | $6.02 \times 10^{23} \text{ mol}^{-1}$ |
| Gas constant | R | $8.31 \text{ J K}^{-1} \text{ mol}^{-1}$ |
| Molar volume of an ideal gas at STP | V_m | $2.27 \times 10^{-2} \text{ m}^3 \text{ mol}^{-1} = 22.7 \text{ dm}^3 \text{ mol}^{-1}$ |
| Specific heat capacity of water | c_w | $4.18 \text{ kJ kg}^{-1} \text{ K}^{-1} = 4.18 \text{ J g}^{-1} \text{ K}^{-1}$ |
| Ionic product constant for water at 298.15 K | K_w | $1.00 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$ |
| Faraday constant | F | $9.65 \times 10^4 \text{ C mol}^{-1}$ |

3. Metric (SI) multipliers

| Prefix | Abbreviation | Value |
|--------|--------------|------------|
| peta | P | 10^{15} |
| tera | T | 10^{12} |
| giga | G | 10^9 |
| mega | M | 10^6 |
| kilo | k | 10^3 |
| hecto | h | 10^2 |
| deca | da | 10^1 |
| deci | d | 10^{-1} |
| centi | c | 10^{-2} |
| milli | m | 10^{-3} |
| micro | μ | 10^{-6} |
| nano | n | 10^{-9} |
| pico | p | 10^{-12} |
| femto | f | 10^{-15} |

4. Unit conversions and standard conditions

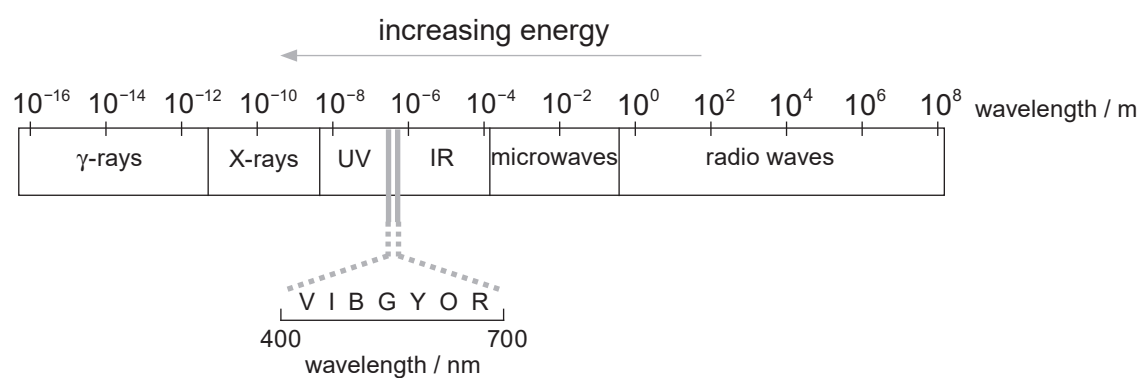
Temperature (K) = temperature (°C) + 273.15

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

STP conditions: 273.15 K and 100 kPa

SATP conditions: 298.15 K and 100 kPa

5. The electromagnetic spectrum



6. Names of the elements

| Element | Symbol | Atomic number |
|--------------|--------|---------------|
| actinium | Ac | 89 |
| aluminium | Al | 13 |
| americium | Am | 95 |
| antimony | Sb | 51 |
| argon | Ar | 18 |
| arsenic | As | 33 |
| astatine | At | 85 |
| barium | Ba | 56 |
| berkelium | Bk | 97 |
| beryllium | Be | 4 |
| bismuth | Bi | 83 |
| bohrium | Bh | 107 |
| boron | B | 5 |
| bromine | Br | 35 |
| cadmium | Cd | 48 |
| caesium | Cs | 55 |
| calcium | Ca | 20 |
| californium | Cf | 98 |
| carbon | C | 6 |
| cerium | Ce | 58 |
| chlorine | Cl | 17 |
| chromium | Cr | 24 |
| cobalt | Co | 27 |
| copper | Cu | 29 |
| curium | Cm | 96 |
| darmstadtium | Ds | 110 |
| dubnium | Db | 105 |

| Element | Symbol | Atomic number |
|-------------|--------|---------------|
| dysprosium | Dy | 66 |
| einsteinium | Es | 99 |
| erbium | Er | 68 |
| europium | Eu | 63 |
| fermium | Fm | 100 |
| flerovium | Fl | 114 |
| fluorine | F | 9 |
| francium | Fr | 87 |
| gadolinium | Gd | 64 |
| gallium | Ga | 31 |
| germanium | Ge | 32 |
| gold | Au | 79 |
| hafnium | Hf | 72 |
| hassium | Hs | 108 |
| helium | He | 2 |
| holmium | Ho | 67 |
| hydrogen | H | 1 |
| indium | In | 49 |
| iodine | I | 53 |
| iridium | Ir | 77 |
| iron | Fe | 26 |
| krypton | Kr | 36 |
| lanthanum | La | 57 |
| lawrencium | Lr | 103 |
| lead | Pb | 82 |
| lithium | Li | 3 |
| livermorium | Lv | 116 |
| lutetium | Lu | 71 |

| Element | Symbol | Atomic number |
|--------------|--------|---------------|
| magnesium | Mg | 12 |
| manganese | Mn | 25 |
| meitnerium | Mt | 109 |
| mendelevium | Md | 101 |
| mercury | Hg | 80 |
| molybdenum | Mo | 42 |
| moscovium | Mc | 115 |
| neodymium | Nd | 60 |
| neon | Ne | 10 |
| neptunium | Np | 93 |
| nickel | Ni | 28 |
| nihonium | Nh | 113 |
| niobium | Nb | 41 |
| nitrogen | N | 7 |
| nobelium | No | 102 |
| oganesson | Og | 118 |
| osmium | Os | 76 |
| oxygen | O | 8 |
| palladium | Pd | 46 |
| phosphorus | P | 15 |
| platinum | Pt | 78 |
| plutonium | Pu | 94 |
| polonium | Po | 84 |
| potassium | K | 19 |
| praseodymium | Pr | 59 |
| promethium | Pm | 61 |
| protactinium | Pa | 91 |
| radium | Ra | 88 |
| radon | Rn | 86 |
| rhenium | Re | 75 |
| rhodium | Rh | 45 |

| Element | Symbol | Atomic number |
|---------------|--------|---------------|
| roentgenium | Rg | 111 |
| rubidium | Rb | 37 |
| ruthenium | Ru | 44 |
| rutherfordium | Rf | 104 |
| samarium | Sm | 62 |
| scandium | Sc | 21 |
| seaborgium | Sg | 106 |
| selenium | Se | 34 |
| silicon | Si | 14 |
| silver | Ag | 47 |
| sodium | Na | 11 |
| strontium | Sr | 38 |
| sulfur | S | 16 |
| tantalum | Ta | 73 |
| technetium | Tc | 43 |
| tellurium | Te | 52 |
| tennessine | Ts | 117 |
| terbium | Tb | 65 |
| thallium | Tl | 81 |
| thorium | Th | 90 |
| thulium | Tm | 69 |
| tin | Sn | 50 |
| titanium | Ti | 22 |
| tungsten | W | 74 |
| uranium | U | 92 |
| vanadium | V | 23 |
| xenon | Xe | 54 |
| ytterbium | Yb | 70 |
| yttrium | Y | 39 |
| zinc | Zn | 30 |
| zirconium | Zr | 40 |

7. The periodic table

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---------------------------|---------------------------|-----------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|
| 1 | 1 H 1.01 | | | | | | | | | | | | | | | | | 2 He 4.00 |
| 2 | 3 Li 6.94 | 4 Be 9.01 | | | | | | | | | | | | | | 8 O 16.00 | 9 F 19.00 | 10 Ne 20.18 |
| 3 | 11 Na 22.99 | 12 Mg 24.31 | | | | | | | | | | | | | | 16 S 32.07 | 17 Cl 35.45 | 18 Ar 39.95 |
| 4 | 19 K 39.10 | 20 Ca 40.08 | 21 Sc 44.96 | 22 Ti 47.87 | 23 V 50.94 | 24 Cr 52.00 | 25 Mn 54.94 | 26 Fe 55.85 | 27 Co 58.93 | 28 Ni 58.69 | 29 Cu 63.55 | 30 Zn 65.38 | 31 Ga 69.72 | 32 Ge 72.63 | 33 As 74.92 | 34 Se 78.96 | 35 Br 79.90 | 36 Kr 83.80 |
| 5 | 37 Rb 85.47 | 38 Sr 87.62 | 39 Y 88.91 | 40 Zr 91.22 | 41 Nb 92.91 | 42 Mo 95.96 | 43 Tc (98) | 44 Ru 101.07 | 45 Rh 102.91 | 46 Pd 106.42 | 47 Ag 107.87 | 48 Cd 112.41 | 49 In 114.82 | 50 Sn 118.71 | 51 Sb 121.76 | 52 Te 127.60 | 53 I 126.90 | 54 Xe 131.29 |
| 6 | 55 Cs 132.91 | 56 Ba 137.33 | 57 La † 138.91 | 72 Hf 178.49 | 73 Ta 180.95 | 74 W 183.84 | 75 Re 186.21 | 76 Os 190.23 | 77 Ir 192.22 | 78 Pt 195.08 | 79 Au 196.97 | 80 Hg 200.59 | 81 Tl 204.38 | 82 Pb 207.20 | 83 Bi 208.98 | 84 Po (209) | 85 At (210) | 86 Rn (222) |
| 7 | 87 Fr (223) | 88 Ra (226) | 89 Ac ‡ (227) | 104 Rf (267) | 105 Db (268) | 106 Sg (269) | 107 Bh (270) | 108 Hs (269) | 109 Mt (278) | 110 Ds (281) | 111 Rg (281) | 112 Cn (285) | 113 Nh (286) | 114 Fl (289) | 115 Mc (288) | 116 Lv (293) | 117 Ts (294) | 118 Og (294) |
| | | | † | | | | | | | | | | | | | | | |
| | | | ‡ | | | | | | | | | | | | | | | |
| | | | | 58 Ce 140.12 | 59 Pr 140.91 | 60 Nd 144.24 | 61 Pm (145) | 62 Sm 150.36 | 63 Eu 151.96 | 64 Gd 157.25 | 65 Tb 158.93 | 66 Dy 162.50 | 67 Ho 164.93 | 68 Er 167.26 | 69 Tm 168.93 | 70 Yb 173.05 | 71 Lu 174.97 | |
| | | | | 90 Th 232.04 | 91 Pa 231.04 | 92 U 238.03 | 93 Np (237) | 94 Pu (244) | 95 Am (243) | 96 Cm (247) | 97 Bk (247) | 98 Cf (251) | 99 Es (252) | 100 Fm (257) | 101 Md (258) | 102 No (259) | 103 Lr (262) | |

10. Atomic and ionic radii of the elements

The values for atomic radii used in this table are the covalent radii of the elements.

| | | Atomic radius / 10^{-12} m | | | | | | | | | | | | | | | | 37 He |
|------------------------------|------------------------------|--------------------------------------|---|---|--|---|---|---|--|---|--|---|---|------------------------------|------------------------------|-----------------------------|--|------------------------------|
| | | Element | | | | | | | | | | | | | | | | |
| | | Ionic radius / 10^{-12} m (charge) | | | | | | | | | | | | | | | | |
| 32 H | | | | | | | | | | | | | | | | | | |
| 130 Li 76 (1+) | 99 Be 45 (2+) | | | | | | | | | | | | | | | | | 60 F 133 (1-) |
| 160 Na 102 (1+) | 140 Mg 72 (2+) | | | | | | | | | | | | | | | | | 100 Cl 181 (1-) |
| 200 K 138 (1+) | 174 Ca 100 (2+) | 159 Sc 75 (3+) | 148 Ti 86 (2+) 61 (4+) | 144 V 79 (2+) 54 (5+) | 130 Cr 62 (3+) 44 (6+) | 129 Mn 83 (2+) 53 (4+) | 124 Fe 61 (2+) 55 (3+) | 118 Co 65 (2+) 55 (3+) | 117 Ni 69 (2+) | 122 Cu 77 (1+) 73 (2+) | 120 Zn 74 (2+) | 123 Ga 62 (3+) | 120 Ge 53 (4+) 272 (4-) | 118 Se 198 (2-) | 117 Br 196 (1-) | 116 Kr | | |
| 215 Rb 152 (1+) | 190 Sr 118 (2+) | 176 Y 90 (3+) | 164 Zr 72 (4+) | 156 Nb 72 (3+) 64 (5+) | 146 Mo 65 (4+) | 138 Tc 65 (4+) | 136 Ru 68 (3+) 62 (4+) | 134 Rh 67 (3+) 60 (4+) | 130 Pd 86 (2+) 62 (4+) | 136 Ag 115 (1+) | 140 Cd 95 (2+) | 142 In 80 (+3) | 140 Sn 118 (2+) 69 (4+) | 137 Te 221 (2-) | 136 I 220 (1-) | 136 Xe | | |
| 238 Cs 167 (1+) | 206 Ba 135 (2+) | 194 La † 103 (3+) | 164 Hf 71 (4+) | 158 Ta 64 (5+) | 150 W 66 (4+) 60 (6+) | 141 Re 63 (4+) 53 (7+) | 136 Os 63 (4+) 55 (6+) | 132 Ir 68 (3+) 63 (4+) | 130 Pt 80 (2+) 63 (4+) | 130 Au 137 (1+) 85 (3+) | 132 Hg 119 (1+) 102 (2+) | 144 Tl 150 (1+) 89 (3+) | 145 Pb 119 (2+) 78 (4+) | 142 Po 97 (4+) | 148 At | 146 Rn | | |
| 242 Fr | 211 Ra | 201 Ac ‡ | | | | | | | | | | | | | | | | |
| | | † | 184 Ce 101 (3+) 87 (4+) | 190 Pr 99 (3+) 85 (4+) | 188 Nd 98 (3+) | 186 Pm 97 (3+) | 185 Sm 96 (3+) | 183 Eu 117 (2+) 95 (3+) | 182 Gd 94 (3+) | 181 Tb 92 (3+) 76 (4+) | 180 Dy 91 (3+) | 179 Ho 90 (+3) | 177 Er 89 (3+) | 177 Tm 88 (3+) | 178 Yb 87 (3+) | 174 Lu 86 (3+) | | |
| | | ‡ | 190 Th 94 (4+) | 184 Pa 104 (3+) 90 (4+) | 183 U 89 (4+) 73 (6+) | 180 Np 101 (3+) 87 (4+) | 180 Pu 100 (3+) 86 (4+) | 173 Am 98 (3+) 85 (4+) | 168 Cm 97 (3+) | 168 Bk 96 (3+) | 168 Cf 95 (3+) | 165 Es | 167 Fm | 173 Md | 176 No 110 (2+) | 161 Lr | | |

11. Covalent or average covalent bond lengths

Single bonds

| Bond | Length / 10^{-12} m | Bond | Length / 10^{-12} m | Bond | Length / 10^{-12} m | Bond | Length / 10^{-12} m |
|--------|-----------------------|--------|-----------------------|---------|-----------------------|---------|-----------------------|
| H — H | 74 | N — H | 101 | Si — H | 148 | S — H | 134 |
| H — F | 92 | N — N | 146 | Si — Si | 232 | S — S | 205 |
| H — Cl | 128 | N — O | 136 | Si — S | 215 | S — F | 158 |
| H — Br | 141 | N — Si | 174 | Si — F | 156 | S — Cl | 199 |
| H — I | 160 | N — S | 175 | Si — Cl | 202 | S — Br | 227 |
| | | N — F | 136 | Si — Br | 216 | | |
| C — H | 108 | N — Cl | 197 | Si — I | 243 | F — F | 142 |
| C — C | 154 | N — Br | 214 | | | F — Cl | 163 |
| C — N | 147 | | | P — H | 142 | F — Br | 176 |
| C — O | 143 | O — H | 97 | P — P | 221 | F — I | 191 |
| C — Si | 185 | O — O | 148 | P — S | 210 | | |
| C — P | 184 | O — Si | 163 | P — F | 154 | Cl — Cl | 199 |
| C — S | 182 | O — P | 154 | P — Cl | 203 | Cl — Br | 214 |
| C — F | 138 | O — S | 161 | P — Br | 220 | Cl — I | 232 |
| C — Cl | 177 | O — F | 142 | P — I | 247 | | |
| C — Br | 194 | O — Cl | 170 | | | Br — Br | 228 |
| C — I | 214 | | | | | Br — I | 247 |
| | | | | | | | |
| | | | | | | I — I | 267 |

Multiple bonds

| Bond | Length / 10^{-12} m | Bond | Length / 10^{-12} m | Bond | Length / 10^{-12} m |
|--------------|-----------------------|--------------|-----------------------|-------|-----------------------|
| C = C | 134 | N = N | 125 | O = O | 121 |
| C = N | 130 | N = O | 114 | O = S | 143 |
| C = O | 122 | | | | |
| C = S | 156 | | | S = S | 189 |
| | | | | | |
| C \equiv C | 120 | N \equiv N | 110 | | |
| C \equiv N | 116 | | | | |
| C \equiv O | 113 | | | | |

12. Bond enthalpies or average bond enthalpies at 298.15 K

Single bonds

| Bond | Enthalpy / kJ mol^{-1} | Bond | Enthalpy / kJ mol^{-1} | Bond | Enthalpy / kJ mol^{-1} | Bond | Enthalpy / kJ mol^{-1} |
|--------|---------------------------------|--------|---------------------------------|---------|---------------------------------|---------|---------------------------------|
| H — H | 436 | N — H | 391 | Si — H | 323 | S — H | 364 |
| H — F | 567 | N — N | 158 | Si — Si | 226 | S — S | 266 |
| H — Cl | 431 | N — O | 214 | Si — S | 293 | S — F | 327 |
| H — Br | 366 | N — F | 278 | Si — F | 597 | S — Cl | 271 |
| H — I | 298 | N — Cl | 192 | Si — Cl | 400 | S — Br | 218 |
| | | | | Si — Br | 330 | | |
| C — H | 414 | O — H | 463 | Si — I | 234 | F — F | 159 |
| C — C | 346 | O — O | 144 | | | F — Cl | 255 |
| C — N | 286 | O — Si | 466 | P — H | 322 | F — Br | 249 |
| C — O | 358 | O — P | 363 | P — P | 198 | F — I | 280 |
| C — Si | 307 | O — F | 191 | P — F | 490 | | |
| C — P | 264 | O — Cl | 206 | P — Cl | 322 | Cl — Cl | 242 |
| C — S | 289 | O — Br | 201 | P — Br | 264 | Cl — Br | 219 |
| C — F | 492 | O — I | 201 | P — I | 184 | Cl — I | 211 |
| C — Cl | 324 | | | | | | |
| C — Br | 285 | | | | | Br — Br | 193 |
| C — I | 228 | | | | | Br — I | 178 |
| | | | | | | | |
| | | | | | | I — I | 151 |

Multiple bonds

| Bond | Enthalpy / kJ mol^{-1} | Bond | Enthalpy / kJ mol^{-1} | Bond | Enthalpy / kJ mol^{-1} |
|--------------|---------------------------------|--------------|---------------------------------|-------|---------------------------------|
| C = C | 614 | N = N | 470 | O = O | 498 |
| C = N | 615 | N = O | 587 | O = S | 522 |
| C = O | 804 | | | | |
| C = S | 536 | | | S = S | 429 |
| | | | | | |
| C \equiv C | 839 | N \equiv N | 945 | | |
| C \equiv N | 890 | | | | |
| C \equiv O | 1077 | | | | |

13. Thermodynamic data (selected compounds)

| Substance | Formula | State | $\Delta H_f^\ominus / \text{kJ mol}^{-1}$ | $\Delta G_f^\ominus / \text{kJ mol}^{-1}$ | $S^\ominus / \text{J K}^{-1} \text{mol}^{-1}$ |
|-------------------------|---|-------|---|---|---|
| methane | CH ₄ | g | -74 | -50 | +186 |
| ethane | C ₂ H ₆ | g | -84 | -32 | +230 |
| propane | C ₃ H ₈ | g | -105 | -24 | +270 |
| butane | C ₄ H ₁₀ | g | -126 | -17 | +310 |
| pentane | C ₅ H ₁₂ | l | -173 | | |
| hexane | C ₆ H ₁₄ | l | -199 | | |
| ethene | C ₂ H ₄ | g | +52 | +68 | +220 |
| propene | C ₃ H ₆ | g | +20 | +62 | +267 |
| but-1-ene | C ₄ H ₈ | g | +0.1 | +71 | +306 |
| <i>cis</i> -but-2-ene | C ₄ H ₈ | g | -7 | +66 | +301 |
| <i>trans</i> -but-2-ene | C ₄ H ₈ | g | -11 | +63 | +297 |
| ethyne | C ₂ H ₂ | g | +228 | +211 | +201 |
| propyne | C ₃ H ₄ | g | +185 | +194 | +248 |
| buta-1,3-diene | C ₄ H ₆ | g | +110 | +151 | +279 |
| cyclohexane | C ₆ H ₁₂ | l | -156 | | |
| benzene | C ₆ H ₆ | l | +49 | +125 | +173 |
| methylbenzene | C ₆ H ₅ CH ₃ | l | +12 | | |
| ethylbenzene | C ₆ H ₅ CH ₂ CH ₃ | l | -12 | | |
| phenylethene | C ₆ H ₅ CHCH ₂ | l | +104 | | |
| chloromethane | CH ₃ Cl | g | -82 | -58 | +235 |
| dichloromethane | CH ₂ Cl ₂ | l | -124 | | +178 |
| trichloromethane | CHCl ₃ | l | -134 | -74 | +202 |
| bromomethane | CH ₃ Br | g | -36 | -26 | +246 |
| iodomethane | CH ₃ I | l | -14 | | +163 |
| chloroethane | C ₂ H ₅ Cl | g | -137 | -53 | |
| bromoethane | C ₂ H ₅ Br | l | -90 | -26 | +199 |
| chlorobenzene | C ₆ H ₅ Cl | l | +11 | | |
| methanol | CH ₃ OH | l | -239 | -167 | +127 |
| ethanol | C ₂ H ₅ OH | l | -278 | -175 | +161 |
| phenol | C ₆ H ₅ OH | s | -165 | | +144 |
| methanal | HCHO | g | -109 | -102 | +219 |
| ethanal | CH ₃ CHO | g | -166 | -133 | +264 |
| propanone | (CH ₃) ₂ CO | l | -248 | | +200 |
| methanoic acid | HCOOH | l | -425 | -361 | +129 |
| ethanoic acid | CH ₃ COOH | l | -484 | -390 | +160 |
| benzoic acid | C ₆ H ₅ COOH | s | -385 | | +168 |
| methylamine | CH ₃ NH ₂ | g | -23 | +32 | +243 |
| water | H ₂ O | l | -286 | -237 | +70 |
| steam | H ₂ O | g | -242 | -229 | +189 |
| carbon monoxide | CO | g | -111 | -137 | +198 |
| carbon dioxide | CO ₂ | g | -394 | -394 | +214 |
| hydrogen bromide | HBr | g | -36 | -53 | +199 |
| hydrogen chloride | HCl | g | -92 | -95 | +187 |
| hydrogen fluoride | HF | g | -273 | -275 | +174 |
| hydrogen iodide | HI | g | +26 | +2 | +207 |

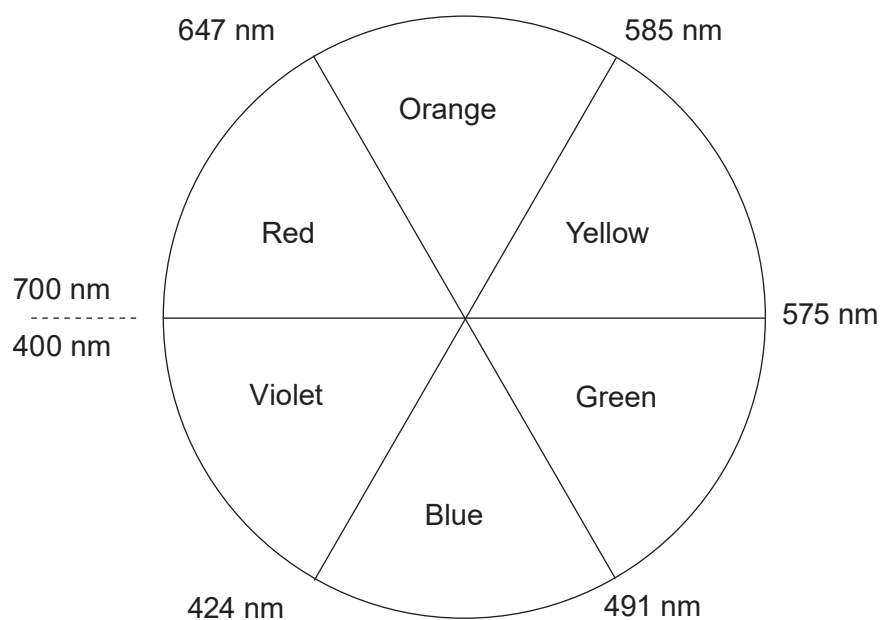
14. Enthalpies of combustion

The values of the molar enthalpy of combustion (ΔH_c^\ominus) in the following table refer to a temperature of 298.15 K and a pressure of 100 kPa.

| Substance | Formula | State | $\Delta H_c^\ominus / \text{kJ mol}^{-1}$ |
|-------------------|---|-------|---|
| hydrogen | H ₂ | g | -286 |
| sulfur | S | s | -297 |
| carbon (graphite) | C | s | -394 |
| carbon monoxide | CO | g | -283 |
| methane | CH ₄ | g | -891 |
| ethane | C ₂ H ₆ | g | -1561 |
| propane | C ₃ H ₈ | g | -2219 |
| butane | C ₄ H ₁₀ | g | -2878 |
| pentane | C ₅ H ₁₂ | l | -3509 |
| hexane | C ₆ H ₁₄ | l | -4163 |
| octane | C ₈ H ₁₈ | l | -5470 |
| cyclohexane | C ₆ H ₁₂ | l | -3920 |
| ethene | C ₂ H ₄ | g | -1411 |
| buta-1,3-diene | C ₄ H ₆ | g | -2541 |
| ethyne | C ₂ H ₂ | g | -1301 |
| benzene | C ₆ H ₆ | l | -3268 |
| methylbenzene | C ₆ H ₅ CH ₃ | l | -3910 |
| naphthalene | C ₁₀ H ₈ | s | -5156 |
| chloroethane | C ₂ H ₅ Cl | g | -1413 |
| iodoethane | C ₂ H ₅ I | l | -1463 |
| trichloromethane | CHCl ₃ | l | -473 |
| methanol | CH ₃ OH | l | -726 |
| ethanol | C ₂ H ₅ OH | l | -1367 |

| Substance | Formula | State | $\Delta H_c^\ominus / \text{kJ mol}^{-1}$ |
|------------------|--|-------|---|
| propan-1-ol | C ₃ H ₇ OH | l | -2021 |
| butan-1-ol | C ₄ H ₉ OH | l | -2676 |
| cyclohexanol | C ₆ H ₁₁ OH | s | -3728 |
| phenol | C ₆ H ₅ OH | s | -3053 |
| ethoxyethane | (C ₂ H ₅) ₂ O | l | -2724 |
| methanal | HCHO | g | -571 |
| ethanal | CH ₃ CHO | g | -1167 |
| benzaldehyde | C ₆ H ₅ CHO | l | -3525 |
| propanone | (CH ₃) ₂ CO | l | -1790 |
| pentan-3-one | (C ₂ H ₅) ₂ CO | l | -3100 |
| phenylethanone | CH ₃ COC ₆ H ₅ | l | -4149 |
| methanoic acid | HCOOH | l | -255 |
| ethanoic acid | CH ₃ COOH | l | -874 |
| benzoic acid | C ₆ H ₅ COOH | s | -3228 |
| ethanedioic acid | (COOH) ₂ | s | -243 |
| ethyl ethanoate | CH ₃ COOC ₂ H ₅ | l | -2238 |
| ethanamide | CH ₃ CONH ₂ | s | -1186 |
| methylamine | CH ₃ NH ₂ | g | -1086 |
| phenylamine | C ₆ H ₅ NH ₂ | l | -3393 |
| nitrobenzene | C ₆ H ₅ NO ₂ | l | -3088 |
| urea | CO(NH ₂) ₂ | s | -633 |
| glucose | C ₆ H ₁₂ O ₆ | s | -2803 |
| sucrose | C ₁₂ H ₂₂ O ₁₁ | s | -5640 |

15. Colour wheel with wavelengths of the visible spectrum



16. Lattice enthalpies at 298.15 K (experimental values)

The lattice enthalpy values ($\Delta H_{\text{lattice}}^{\ominus}$) in the following tables relate to the endothermic process $M_aX_b(s) \rightarrow aM^{b+}(g) + bX^{a-}(g)$ in which the gaseous ions of a crystal are separated to an infinite distance from each other.

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

| Alkali metal halides | $\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$ | | | |
|----------------------|--|-----|-----|-----|
| | F | Cl | Br | I |
| Li | 1049 | 864 | 820 | 764 |
| Na | 930 | 790 | 754 | 705 |
| K | 829 | 720 | 691 | 650 |
| Rb | 795 | 695 | 668 | 632 |
| Cs | 759 | 670 | 647 | 613 |

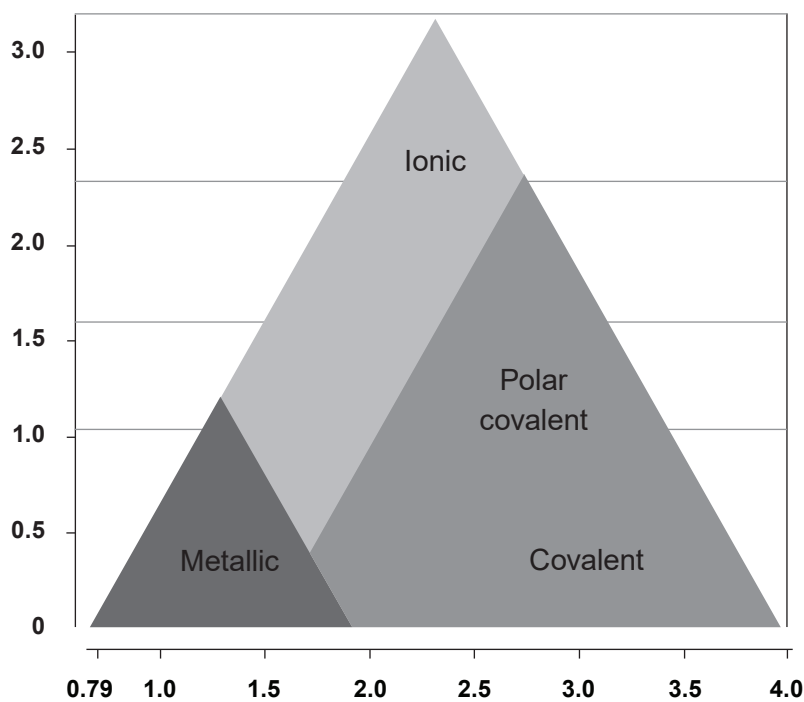
| Other substances | $\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$ |
|-------------------|--|
| CaF ₂ | 2651 |
| BeCl ₂ | 3033 |
| MgCl ₂ | 2540 |
| CaCl ₂ | 2271 |
| SrCl ₂ | 2170 |
| BaCl ₂ | 2069 |
| MgO | 3791 |
| CaO | 3401 |

| Other substances | $\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$ |
|-------------------|--|
| SrO | 3223 |
| BaO | 3054 |
| CuCl ₂ | 2824 |
| AgF | 974 |
| AgCl | 918 |
| AgBr | 905 |
| AgI | 892 |

17. Triangular bonding diagram (van Arkel–Ketelaar triangle)

Electronegativity difference:

$$\Delta\chi = |\chi_a - \chi_b|$$



%
covalent

%
ionic

Average electronegativity:

$$\Sigma\chi = \frac{(\chi_a + \chi_b)}{2}$$

18. Acid–base indicators

| Indicator | pK_a | pH range | Colour change | |
|-------------------|--------|----------|---------------|--------|
| | | | Acid | Alkali |
| methyl orange | 3.7 | 3.1–4.4 | red | yellow |
| bromophenol blue | 4.2 | 3.0–4.6 | yellow | blue |
| bromocresol green | 4.7 | 4.0–5.6 | yellow | blue |
| methyl red | 5.1 | 4.4–6.2 | red | yellow |
| bromothymol blue | 7.0 | 6.0–7.6 | yellow | blue |
| phenol red | 7.9 | 6.4–8.0 | yellow | red |
| phenolphthalein | 9.6 | 8.0–10.0 | colourless | pink |

19. Standard reduction potentials at 298.15 K

| Oxidized species | Reduced species | E^\ominus / V |
|---|--|------------------------|
| $\text{Li}^+(\text{aq}) + \text{e}^-$ | $\rightleftharpoons \text{Li}(\text{s})$ | -3.04 |
| $\text{K}^+(\text{aq}) + \text{e}^-$ | $\rightleftharpoons \text{K}(\text{s})$ | -2.93 |
| $\text{Ca}^{2+}(\text{aq}) + 2\text{e}^-$ | $\rightleftharpoons \text{Ca}(\text{s})$ | -2.87 |
| $\text{Na}^+(\text{aq}) + \text{e}^-$ | $\rightleftharpoons \text{Na}(\text{s})$ | -2.71 |
| $\text{Mg}^{2+}(\text{aq}) + 2\text{e}^-$ | $\rightleftharpoons \text{Mg}(\text{s})$ | -2.37 |
| $\text{Al}^{3+}(\text{aq}) + 3\text{e}^-$ | $\rightleftharpoons \text{Al}(\text{s})$ | -1.66 |
| $\text{Mn}^{2+}(\text{aq}) + 2\text{e}^-$ | $\rightleftharpoons \text{Mn}(\text{s})$ | -1.18 |
| $\text{H}_2\text{O}(\text{l}) + \text{e}^-$ | $\rightleftharpoons \frac{1}{2}\text{H}_2(\text{g}) + \text{OH}^-(\text{aq})$ | -0.83 |
| $\text{Zn}^{2+}(\text{aq}) + 2\text{e}^-$ | $\rightleftharpoons \text{Zn}(\text{s})$ | -0.76 |
| $\text{Fe}^{2+}(\text{aq}) + 2\text{e}^-$ | $\rightleftharpoons \text{Fe}(\text{s})$ | -0.45 |
| $\text{Ni}^{2+}(\text{aq}) + 2\text{e}^-$ | $\rightleftharpoons \text{Ni}(\text{s})$ | -0.26 |
| $\text{Sn}^{2+}(\text{aq}) + 2\text{e}^-$ | $\rightleftharpoons \text{Sn}(\text{s})$ | -0.14 |
| $\text{Pb}^{2+}(\text{aq}) + 2\text{e}^-$ | $\rightleftharpoons \text{Pb}(\text{s})$ | -0.13 |
| $\text{H}^+(\text{aq}) + \text{e}^-$ | $\rightleftharpoons \frac{1}{2}\text{H}_2(\text{g})$ | 0.00 |
| $\text{Cu}^{2+}(\text{aq}) + \text{e}^-$ | $\rightleftharpoons \text{Cu}^+(\text{aq})$ | +0.15 |
| $\text{SO}_4^{2-}(\text{aq}) + 4\text{H}^+(\text{aq}) + 2\text{e}^-$ | $\rightleftharpoons \text{H}_2\text{SO}_3(\text{aq}) + \text{H}_2\text{O}(\text{l})$ | +0.17 |
| $\text{Cu}^{2+}(\text{aq}) + 2\text{e}^-$ | $\rightleftharpoons \text{Cu}(\text{s})$ | +0.34 |
| $\frac{1}{2}\text{O}_2(\text{g}) + \text{H}_2\text{O}(\text{l}) + 2\text{e}^-$ | $\rightleftharpoons 2\text{OH}^-(\text{aq})$ | +0.40 |
| $\text{Cu}^+(\text{aq}) + \text{e}^-$ | $\rightleftharpoons \text{Cu}(\text{s})$ | +0.52 |
| $\frac{1}{2}\text{I}_2(\text{s}) + \text{e}^-$ | $\rightleftharpoons \text{I}^-(\text{aq})$ | +0.54 |
| $\text{Fe}^{3+}(\text{aq}) + \text{e}^-$ | $\rightleftharpoons \text{Fe}^{2+}(\text{aq})$ | +0.77 |
| $\text{Ag}^+(\text{aq}) + \text{e}^-$ | $\rightleftharpoons \text{Ag}(\text{s})$ | +0.80 |
| $\frac{1}{2}\text{Br}_2(\text{l}) + \text{e}^-$ | $\rightleftharpoons \text{Br}^-(\text{aq})$ | +1.09 |
| $\frac{1}{2}\text{O}_2(\text{g}) + 2\text{H}^+(\text{aq}) + 2\text{e}^-$ | $\rightleftharpoons \text{H}_2\text{O}(\text{l})$ | +1.23 |
| $\text{Cr}_2\text{O}_7^{2-}(\text{aq}) + 14\text{H}^+(\text{aq}) + 6\text{e}^-$ | $\rightleftharpoons 2\text{Cr}^{3+}(\text{aq}) + 7\text{H}_2\text{O}(\text{l})$ | +1.36 |
| $\frac{1}{2}\text{Cl}_2(\text{g}) + \text{e}^-$ | $\rightleftharpoons \text{Cl}^-(\text{aq})$ | +1.36 |
| $\text{MnO}_4^-(\text{aq}) + 8\text{H}^+(\text{aq}) + 5\text{e}^-$ | $\rightleftharpoons \text{Mn}^{2+}(\text{aq}) + 4\text{H}_2\text{O}(\text{l})$ | +1.51 |
| $\frac{1}{2}\text{F}_2(\text{g}) + \text{e}^-$ | $\rightleftharpoons \text{F}^-(\text{aq})$ | +2.87 |

20. Infrared data

Characteristic ranges for infrared absorption due to stretching vibrations in organic molecules

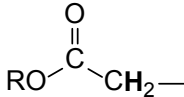
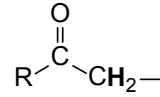
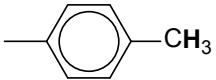
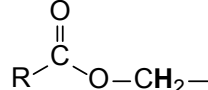
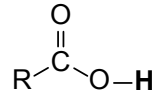
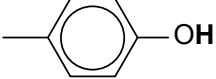

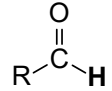
| Bond | Types of organic molecules | Wavenumber / cm^{-1} | Intensity |
|--------------|---|-------------------------------|-----------------------------|
| C — I | iodoalkanes | 490–620 | strong |
| C — Br | bromoalkanes | 500–600 | strong |
| C — Cl | chloroalkanes | 600–800 | strong |
| C — F | fluoroalkanes | 1000–1400 | strong |
| C — O | alcohols, esters, ethers | 1050–1410 | strong |
| C = C | alkenes | 1620–1680 | medium-weak; multiple bands |
| C = O | aldehydes, ketones, carboxylic acids and esters | 1700–1750 | strong |
| C \equiv C | alkynes | 2100–2260 | variable |
| O — H | carboxylic acids (with hydrogen bonding) | 2500–3000 | strong, very broad |
| C — H | alkanes, alkenes, arenes | 2850–3090 | strong |
| O — H | alcohols and phenols (with hydrogen bonding) | 3200–3600 | strong, broad |
| N — H | primary amines | 3300–3500 | medium; two bands |

21. ^1H NMR data

Typical proton chemical shift values (δ) relative to tetramethylsilane (TMS)

R represents an alkyl group, and Hal represents F, Cl, Br or I.

These values may vary for different solvents and conditions.

| Type of proton | Chemical shift / ppm |
|---|----------------------|
| $-\text{CH}_3$ | 0.9–1.0 |
| $-\text{CH}_2-\text{R}$ | 1.3–1.4 |
| $-\text{CHR}_2$ | 1.5 |
|  | 2.0–2.5 |
|  | 2.2–2.7 |
|  | 2.5–3.5 |
| $-\text{C}\equiv\text{C}-\text{H}$ | 1.8–3.1 |
| $-\text{CH}_2-\text{Hal}$ | 3.5–4.4 |
| $\text{R}-\text{O}-\text{CH}_2-$ | 3.3–3.7 |
|  | 3.7–4.8 |
|  | 9.0–13.0 |
| $\text{R}-\text{O}-\text{H}$ | 1.0–6.0 |
| $-\text{CH}=\text{CH}_2$ | 4.5–6.0 |
|  | 4.0–12.0 |
|  | 6.9–9.0 |
|  | 9.4–10.0 |

22. Mass spectral fragments lost

| Mass lost (M_r) | Possible neutral fragment lost |
|---------------------|---------------------------------------|
| 15 | •CH ₃ |
| 17 | •OH |
| 18 | H ₂ O |
| 28 | CH ₂ =CH ₂ CO |
| 29 | •CH ₂ CH ₃ •CHO |
| 31 | •OCH ₃ |
| 45 | •COOH |

23. Uncertainties

| | |
|------------------------|---|
| If: $y = a \pm b$ | then: $\Delta y = \Delta a + \Delta b$ |
| If: $y = \frac{ab}{c}$ | then: $\frac{\Delta y}{y} = \frac{\Delta a}{a} + \frac{\Delta b}{b} + \frac{\Delta c}{c}$ |
| If: $y = a^n$ | then: $\frac{\Delta y}{y} = \left n \frac{\Delta a}{a} \right $ |

24. References

Data in sections 7, 8, 9, 10, 11, 12, 13, 14, 16, 18, 19, 20, 21 and 22 were taken fully or in part from:

Blackman, A., Gahan, L. R., Aylward, G. H., & Findlay, T. J. V. (2014). *Aylward and Findlay's SI Chemical Data*. (7th ed.). John Wiley & Sons.

National Institute of Standards and Technology. (2021). *NIST Chemistry WebBook SRD 69, NIST Standard Reference Database*. U.S. Department of Commerce. <http://webbook.nist.gov>

Rumble, J. R. (Ed.). (2019). *CRC Handbook of Chemistry and Physics*. (100th ed.). CRC Press.

Data in section 17 are reproduced with permission from the author:

Leach, M. R. (2021). *The Chemogenesis Web Book: Timeline of structural theory*. http://www.meta-synthesis.com/webbook/30_timeline/timeline.html

Updates to the publication

This section outlines the updates made to this publication over the past two years. The changes are ordered from the most recent to the oldest updates. Minor spelling and typographical corrections are not listed.

Changes for February 2024

11. Covalent or average covalent bond lengths

The bond length for F — I was corrected to 191×10^{-12} m.

18. Acid–base indicators

The pH ranges for bromocresol green, phenol red and phenolphthalein were updated according to the latest published data.

23. Uncertainties

This section listing uncertainties propagation formulae was added.