AQA Formulae

Atomic Structure

Fundamental Particles

number of neutrons = mass number – atomic number

Time of Flight Mass Spectroscopy

Relative atomic mass = (mass of isotope 1 x abundance of isotope 1) + (mass of isotope 2 x abundance of isotope 2)/100

$E_k = ½mv^2$ where m = mass of one ion in kg, v = speed of ion in ms^{-1}

v = d/t where d = distance of tube in m, t = time taken for ion to reach detector in secs

Amount of Substance

% atom economy = M_r of desired product/sum of M_r of all products x 100

% yield = actual mass/theoretical mass x 100

moles = mass/M_r

moles = concentration x volume/1000 (dm^3)

moles = number of particles/6.02×10^{23} (value in data sheet)

PV = nRT (gases) where v is in m^3, T is in K and P is in Pa, R (in data sheet)

density = mass/volume

percentage error = uncertainty in instrument/value x 100

Energetics

ΔH = sum of bonds broken – sum of bonds made (mean bond enthalpies)

Q = mc ΔT where m = mass of water, c = 4.18 (in data sheet) and T is in K

Equilibrium

$$aA + bB \rightleftharpoons cC + dD$$

$$K_c = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

Kinetics (Rates)

Rate = 1/time

Rate = gradient of concentration-time curve

Thermodynamics

ΔS = (sum of entropy of products) – (sum of entropy of reactants)

ΔH = (sum of enthalpy of products) – (sum of enthalpy of reactants)

$$\Delta G = \Delta H - T\Delta S_{system}$$

$$\text{min. temp.} = \Delta H/\Delta S_{system}$$

Equilibrium

Example:

$$CH_4(g) + H_2O(g) \rightleftharpoons CO(g) + 3H_2(g)$$

$$K_p = \frac{p(CO) \times p(H_2)^3}{p(CH_4) \times p(H_2O)}$$

Mole fraction = moles of one gas/moles of all the gases

Partial Pressure = mole fraction x total pressure

Total Pressure = sum of the partial pressures

Electrode Potentials

E_{cell} = $E^{\ominus}$ of the more positive value – $E^{\ominus}$ of the more negative value

or

E_{cell} = $E^{\ominus}$ of the species being reduced – $E^{\ominus}$ of the species being oxidised

Acids and Bases

$$pH = -\log_{10} [H^+]$$

$$[H^+] = 10^{-pH}$$

$K_w = [H^+][OH^-] = 1\times10^{-14}\ mol^2dm^{-6}$ (at room temp) (value in data sheet)

$K_w = [H^+]^2$ (pure water)

Half-equivalence point: $K_a = [H^+]$ or $pK_a = pH$

Expression and use in buffer calculations:

$$K_a = \frac{[H^+][A^-]}{[HA]}$$

Weak acid calculations:

$$K_a = \frac{[H^+]^2}{[HA]}$$

$$pK_a = -\log_{10}K_a$$

$$K_a = 10^{-pKa}$$

Transition Metals

$\Delta E=hv$ where $h = 6.63 \times 10^{-34}$, v = frequency in Hz

$c = v \times \lambda$ where c = speed of light $3 \times 10^8\ ms^{-1}$, λ = wavelength in m

Rates

For $A + B \rightarrow C + D$ rate = $k[A][B]$

Arrhenius: $k = Ae^{-Ea/RT}$

$\ln k = \ln A - E_a/RT$ (both given in data sheet)

Rearranged:

$$E_a = (\ln A - \ln k) \times RT \quad \text{and} \quad T = E_a/(\ln A - \ln k) \times R$$