Calculations in Chemistry

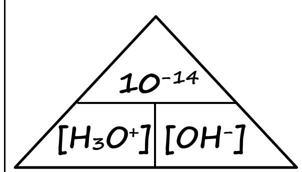
AS 91164 Demonstrate understanding of bonding, structure, properties & energy changes	AS 91166 Demonstrate understanding of chemical reactivity
• exothermic and endothermic reactions including energy (enthalpy) changes associated with differing amounts of substances and changes of state • enthalpy changes associated with the making and breaking of chemical bonds • calculations of energy changes using $\Delta_r H$ and reaction stoichiometry, and bond enthalpy.	• the equilibrium constant (K_c) for homogeneous systems; This may involve calculations (If K_c ↑ eqm position shifts to right, favours the products ….. as bigger [products] ÷ smaller [reactants] = bigger value of K_c . • calculations involving Kw and pH (restricted to strong acids and bases).

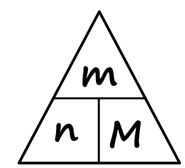
Useful formulae you need to memorise

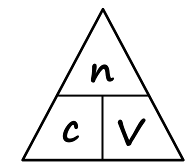
$pH = -\log[H_3O^+]$ $[H_3O^+] = 10^{-pH}$ or inv log (-pH) $K_w = 1 \times 10^{-14} = [H_3O^+][OH^-]$

$n = m/M$ or $m = nM$ (n is amount, in mol, m is mass in g, & M is molar mass, in g mol^{-1}

$n = cV$ (n is amount, in mol, c is conc$^{\underline{n}}$ in mol L^{-1} and V is volume in L







$\Delta H = \Sigma\Delta H(\text{bonds broken}) + \Sigma\Delta H(\text{bonds made})$ - This basically means that you add up all the energies of the broken bonds (+); add up all the energies of the bonds that are reformed (-) and add them to each other. You will be given the bond energies but you MUST remember that bond breaking is endothermic (+ΔH) and bond making is exothermic (-ΔH) E.g. H-H → H + H; +436 kJ while H + H → H_2 ; -436 kJ

Units commonly used

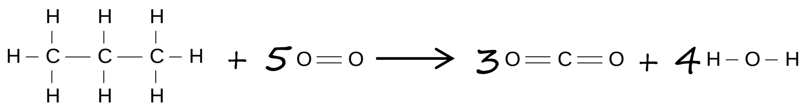
- Energy: J or kJ or J mol^{-1} or kJ mol^{-1} For enthalpy changes the units of kJ mol^{-1} refer to **one mole of the equation as written** rather than with respect to any particular component of the equation.
- Amount of substance: mol (1 mole = 6×10^{23} particles; atoms, molecules, or ions etc.).
- Concentration: mol L^{-1} ; [……] - square brackets mean concentration of …….
- Mass of substance: g or kg
- pH: has NO units
- K_c: has NO units (@ Level 2)

91164	Sample calculations	91166

The complete combustion of propane can be represented by the following equation

$$CH_3CH_2CH_3 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

or we could redraw it to represent the bonds present:



Bond type	Average bond enthalpy kJ mol^{-1}
C-H	413
C-C	347
O=O	498
C=O	805
O-H	464

Break

2x C-C 2x 347
8x C-H 8x 413
5x O=O 5x 498
= 6488 kJ

Make

6x C=O 6x -498
8x O-H 8x -464
= -8542 kJ

ΔH = 6488 + - 8542 = -2054 kJ

Remember "make" is exothermic so −

Calculate the amount of energy released when 25.0 grams of C_4H_{10}(l) is burned in oxygen using the equation provided.

Method 1

$2C_4H_{10}$ (l) + $13O_2$ (g) → $8CO_2$ (g) + $10H_2O$ (g); ΔH = -5315 kJ

2 moles	-5315 kJ
116* g	-5315 kJ
25g	$\frac{25 \times -5315}{116}$
	= -1145.5 kJ

M(C_4H_{10}) = (4 x 12.0) + (10 x 1.00) = 58.0 g mol^{-1}.
So 2 mol has a mass of 116 g

1145.5 kJ of heat would be released.

Method 2

$2C_4H_{10}$ (l) + $13O_2$ (g) → $8CO_2$ (g) + $10H_2O$ (g); ΔH = -5315 kJ

M(C_4H_{10}) = 58.0 g mol^{-1} n(C_4H_{10}) = m/M = 25.0/58.0 = 0.431 mol

If combustion of 2 mol of C_4H_{10} releases 5315 kJ of energy, then the combustion of 0.431 mol of C_4H_{10} releases (0.431/2) x 5315 = 1145.5 kJ (calculated keeping all numbers in calculator and rounding only final answer).

Determine the [H_3O^+], [OH^-] and pH in each of the following solutions.
(a) 0.00112 mol L^{-1} HCl solution.
(b) 3.68×10^{-2} mol L^{-1} NaOH solution.

2 values don't need calculating at all……. HCl is a strong acid, reacts completely with water; HCl + H_2O → H_3O^+ + Cl^- so [H_3O^+] = [HCl]
NaOH is a strong base, dissolves completely in water;
NaOH + aq → Na^+ + OH^- so [OH^-] = [NaOH]

	[H_3O^+]	[OH^-]	pH
(a)	0.00112		
(b)		3.68×10^{-2}	

	[H_3O^+]	[OH^-]	pH
(a)	0.00112	[OH^-] = 10^{-14}/[H_3O^+] = 10^{-14}/ 0.00112 = 8.93×10^{-12}	pH = -log [H_3O^+] pH = -log 0.00112 = 2.95
(b)	[H_3O^+]= 10^{-14}/[OH^-] [H_3O^+]= 10^{-14}/ 3.68×10^{-2} = 2.72×10^{13}	3.68×10^{-2}	pH = -log [H_3O^+] pH = -log = 12.6

Do a quick reality check… yes… an acid with pH of 2.95 and a base with pH of 12.6 sounds fine! ☺

Equilibrium constant (Kc) for homogeneous systems may involve calculations.

e.g. For the reaction: $H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$

$$K_c = \frac{[HI]^2}{[H_2][I_2]}$$

A mixture of hydrogen and iodine was heated in a sealed flask at 491°C and, at equilibrium, the concentration of hydrogen was 2.50×10^{-2} mol L^{-1}, iodine was 2.50×10^{-2} mol L^{-1}, and hydrogen iodide was 1.71×10^{-1} mol L^{-1}. Calculate K_c.

$$K_c = \frac{(1.71 \times 10^{-1})^2}{(2.50 \times 10^{-2}) \times (2.50 \times 10^{-2})} = 46.8 \text{ (no units)}$$