ΔH calculations

CALCULATION OF ENTHALPY CHANGES

The heat involved in changing the temperature of any substance can be calculated from the equation:

Heat energy = mass (m) × specific heat capacity (c) × temperature change (ΔT)

The specific heat capacity of water is 4.18 kJ kg^{-1} K^{-1}. That is, it requires one kilojoule of energy to raise the temperature of one kilogram of water by one kelvin.

Enthalpy changes are normally quoted in kJ mol^{-1}, for either a reactant or a product, so it is also necessary to work out the number of moles involved in the reaction which produces the heat change in the water.

Worked example 1

50.0 cm^3 of 1.00 mol dm^{-3} hydrochloric acid solution was added to 50.0 cm^3 of 1.00 mol dm^{-3} sodium hydroxide solution in a polystyrene beaker. The initial temperature of both solutions was 16.7 °C. After stirring and accounting for heat loss the highest temperature reached was 23.5 °C. Calculate the enthalpy change for this reaction.

Step 1. Write equation for reaction

$HCl(aq) + NaOH(aq) \rightarrow NaCl(aq) + H_2O(l)$

Step 2. Calculate molar quantities

$$\text{Amount of HCl} = \frac{50.0}{1000} \times 1.00 = 5.00 \times 10^{-2}\ \text{mol}$$

$$\text{Amount of NaOH} = \frac{50.0}{1000} \times 1.00 = 5.00 \times 10^{-2}\ \text{mol}$$

Therefore the heat evolved will be for 5.00×10^{-2} mol

Step 3. Calculate heat evolved

Total volume of solution = 50.0 + 50.0 = 100 cm^3
Assume the solution has the same density and specific heat capacity as water then
mass of 'water' = 100 g = 0.100 kg
Temperature change = 23.5 – 16.7 = 6.8 °C = 6.8 K
Heat evolved in reaction = $0.100 \times 4.18 \times 6.8 = 2.84$ kJ
= 2.84 kJ (for 5.00×10^{-2} mol)

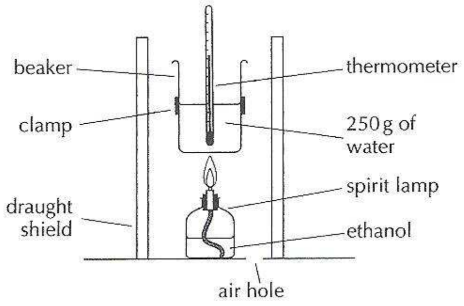
$$\Delta H \text{ for reaction} = -2.84 \times \frac{1}{5.00 \times 10^{-2}} = -56.8\ \text{kJ mol}^{-1}$$

(negative value as the reaction is exothermic)

Worked example 2

A student used a simple calorimeter to determine the enthalpy change for the combustion of ethanol.

$C_2H_5OH(l) + 3O_2(g) \rightarrow 2CO_2(g) + 3H_2O(l)$



When 0.690 g (0.015 mol) of ethanol was burned it produced a temperature rise of 13.2 K in 250 g of water. Calculate ΔH for the reaction.

$$\text{Heat evolved by 0.015 mol} = \frac{250}{1000} \times 4.18 \times 13.2 = 13.79\ \text{kJ}$$

$$\Delta H = -13.79 \times \frac{1}{0.015} = -920\ \text{kJ mol}^{-1}$$

Note: the Data Book value is –1371 kJ mol^{-1}. Reasons for the discrepancy include the fact that not all the heat produced is transferred to the water, the water loses some heat to the surroundings, and there is incomplete combustion of the ethanol.

Worked example 3

50.0 cm^3 of 0.200 mol dm^{-3} copper(II) sulfate solution was placed in a polystyrene cup. After two minutes 1.20 g of powdered zinc was added. The temperature was taken every 30 seconds and the following graph obtained. Calculate the enthalpy change for the reaction taking place.

Step 1. Write the equation for the reaction

$Cu^{2+}(aq) + Zn(s) \rightarrow Cu(s) + Zn^{2+}(aq)$

Step 2. Determine the limiting reagent

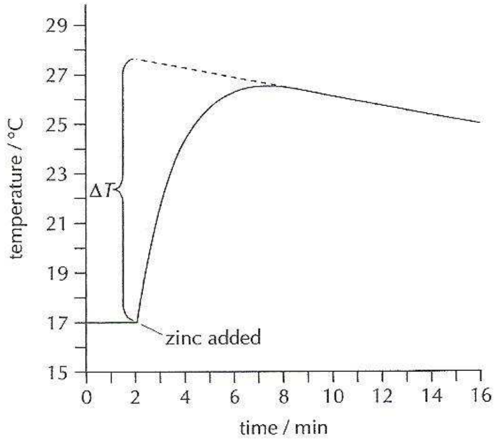
Amount of $Cu^{2+}(aq)$ = 50.0/1000 × 0.200 = 0.0100 mol

Amount of Zn(s) = 1.20/65.37 = 0.0184 mol

$\therefore$ $Cu^{2+}(aq)$ is the limiting reagent

Step 3. Extrapolate the graph (*already done*) to compensate for heat loss and determine ΔT

$\Delta T = 10.4$ °C



Step 4. Calculate the heat evolved in the experiment for 0.0100 mol of reactants

Heat evolved = 50.0/1000 × 4.18 × 10.4 °C = 2.17 kJ

Step 5. Express this as the enthalpy change for the reaction $\Delta H = -2.17 \times \frac{1}{0.0100} = -217\ \text{kJ mol}^{-1}$