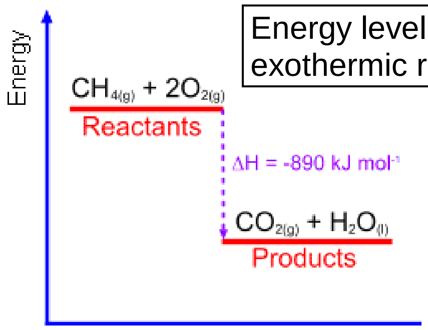
Energetics

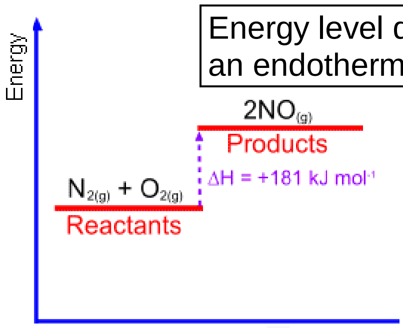
exothermic reactions – heat given out to the surroundings (temperature goes up) (ΔH –ve)

endothermic reactions – heat taken in from the surrounding (temperature goes down) (ΔH +ve)

Energy level diagram for an exothermic reaction



Energy level diagram for an endothermic reaction



Heat energy changes in reactions such as combustion, displacement, dissolving and neutralization can be calculated as: $\boxed{Q = mc\Delta T}$

NOTE: m in this equation is the mass of water heated

Heat energy change = mass x specific heat capacity x temp. change

Molar enthalpy change = heat energy change / no. of moles

Example

Good insulator

100.0 cm^3 of water was measured out and poured into a polystyrene cup. The initial temperature of the water was taken. 5.20 g of ammonium chloride was measured out. The ammonium chloride was added to the water and the solution stirred vigorously until all the ammonium chloride had dissolved. The minimum temperature was recorded.

Initial temperature of water = 18.3 °C **Minimum temperature = 15.1 °C**

Temperature change of the mixture = 3.2 °C

assume that the density of the solution is the same as that of water and so 100.0 cm^3 of solution has a mass of 100.0 g.

$Q = mc\Delta T$ $Q = 100.0 \times 4.18 \times 3.2$ $Q = 1340$ J

Number of moles of NH_4Cl = $\frac{\text{mass}}{\text{Molar mass}} = \frac{5.20}{53.50}$ i.e..0972 mol

Molar mass of NH_4Cl

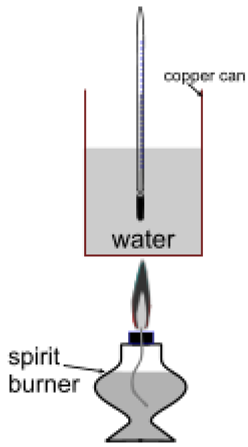
Therefore 1340 J of energy is absorbed when 0.0972 mol NH_4Cl dissolve.

For 1 mole of NH_4Cl dissolving: heat energy absorbed = $\frac{1}{0.0972} \times 1340$ i.e. 13800 J/mol

Therefore the enthalpy change of solution, ΔH_{sol} = +13.8 kJ/mol

Positive, since endothermic.

Example: **When 0.40g of butanol (C_4H_9OH) is burnt the temperature of 200.0 g of water is raised by 12 °C. Calculate the enthalpy change when 1 mole of butanol is burnt.**



Specific heat capacity of water

$Q = mc\Delta T$ $Q = 200.0 \times 4.18 \times 12$ $Q = 10032$ J

Mass of water heated – ***not*** mass of butanol

Number of moles of butanol = $\frac{0.40}{74}$ = 0.0054 mol

Molar mass of butanol

Molar enthalpy change = $\frac{10032}{0.0054}$ = 1855920 J/mol

Molar enthalpy change

ΔH = -1856 kJ/mol

negative, since exothermic.

Reasons the value is less exothermic than expected

some of the heat will be dissipated to the surroundings - not all the heat energy from the burning of the fuel goes to heating up the water and some heats up the surrounding air.

incomplete combustion i.e. some of a hydrocarbon may only be oxidised to CO or C (soot) and not completely oxidised to CO_2.

The enthalpy change of a reaction can be calculated using bond energies

Bond breaking – requires energy – endothermic
Bond making – releases energy – exothermic

Example: the reaction between METHANE and OXYGEN: $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

Combustion is a reaction with oxygen.

Bond energies:

Bond	kJ/mol
C-H	412
C=O	743
O=O	496
O-H	463

BONDS BROKEN:

Bond	Number of bonds	Energy for each bond / kJ/mol	Total energy / kJ/mol
C-H	4	412	1648
O=O	2	496	992
		Grand Total / kJ/mol	2640

Breaking bonds requires energy. ΔH is positive = endothermic

BONDS MADE:

Bond	Number of bonds	Energy for each bond / kJ/mol	Total energy / kJ/mol
C=O	2	743	1486
O-H	4	463	1852
		Grand Total / kJ/mol	3338

Making bonds releases energy. ΔH is negative - exothermic

TOTAL ENERGY CHANGE = BONDS BROKEN - BONDS MADE

Total energy change = 2640 – 3338 ΔH = -698 kJ/mol

The overall process is EXOTHERMIC.

ΔH represents the molar enthalpy change – in this case, the amount of heat given out when 1 mol of CH_4 reacts with 2 mol of O_2.

A chemical reaction will generally be exothermic if more energy is released when bonds are made than is required to break bonds.