IBDP Chemistry

**Topic 5 Energetics**

Notes

5.1 Exothermic and Endothermic Reactions

Vocabulary

**Enthalpy**: energy stored in chemical bonds. It is related to the heat released when bonds are formed. Symbol = H. The change in H is often measured as the change in heat, or ΔH. Enthalpy is measured in units of joules (J) or kilojoules (kJ).

Sometimes enthalpy is written ΔHΘ and the Θ symbol means at **thermochemical standard conditions,** 298 K / 25°C AND 1 atm / 101(.3) kPa (Memorize!). Note: these are NOT the same as stp for gases. stp = 273 K (0 °C) and 1 atm / 101(.3) kPa

Example

2Mg(s) + O2 (g) 🡪 2MgO(s) ΔHΘ = -1200 kJ/mol

This means that 1200 kJ is released when 2 moles Mg react with one mole of O2.

**System**: the chemicals involved in the chemical reaction.

**Surroundings**: everything besides the system.

5.1.1 and 5.1.3

Exothermic reactions release heat and have a negative change in enthalpy, -ΔHΘ, so temperature increases

Endothermic reactions absorb energy from the surroundings and have a positive change in enthalpy (+ΔH°), so temperature decreases OR heat is supplied from another source. Example: boiling water is endothermic, but the temperature remains at about 100 C because heat is supplied by fire.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Heat Flow** | **Sign of *q*** | **Type of Reaction** | **Products** | **Surroundings** |
| from surroundings to system | + (positive) | endothermic | gain energy | lose heat (get colder) |
| from system to surroundings | − (negative) | exothermic | lose energy | gain heat (get hotter) |

5.1.2 Combustion and neutralization reactions are exothermic processes.

Combustion reactions: anything that reacts with oxygen.

CH4 +2 O2 🡪 CO2 + 2H2O ΔHΘ = -804 kJ/mol

Neutralization reaction (or acid-base reaction)

HCl + NaOH 🡪 NaCl + H2O - ΔHΘ

5.1.4 **Energy diagrams**



Is this diagram endothermic or exothermic? Answer: exothermic.

In an exothermic reaction, the enthalpy (“energy” in the diagram should be labeled enthalpy) of products is lower than the reactants.

In an endothermic reaction, the enthalpy of products is higher than reactants.

5.2 Calculations of Enthalpy Changes

5.2.1 When the temperature of a pure substance changes, you can use this equation to measure the change in energy:

Heat energy = m•c•ΔT

m = mass in grams of the substance heated (usually water in a calorimetry experiment).

c = specific heat capacity of the substance heated. For water, c = 4.18 J/g°C

ΔT = final temperature – initial temperature (Celsius)

**Specific** **heat capacity**: the amount of heat (Joules) needed to raise the temperature of one gram of a substance by one degree Celsius. Different materials absorb a different amount of heat when their temperature raises by one degree Celsius. Thus, every material has a different specific heat. Metals usually heat up very easily because they have a low specific heat.

5.2.2 Calorimetry experiments

**Calorimetry** is a technique used to measure the enthalpy of a physical or chemical change.

A calorimeter is a device used to keep heat from escaping to the surroundings. Often, Styrofoam cups are used, which have a very low specific heat, and do not introduce much error. If a different material used, such as copper, then the change in temperature of the calorimeter must be used in the calculation:

Heat absorbed = (m•c•ΔT)liquid + (m•c•ΔT)calorimeter

In a calorimeter, the heat of reaction has the opposite sign of the heat of the calorimeter. (This is because any heat coming *out of* the reaction is going *into* the calorimeter.)

Heat of reaction = - (heat of calorimeter)

5.2.3-4 Calculating enthalpy change from data

Common example: 20.0 cm3 of 2.00 M aqueous sodium hydroxide is added to 30.0 cm3 2.00 M aqueous hydrochloric acid. Total volume = 50.0 cm3. Density of water = 1.00 g/ cm3 Initial temperature = 20.2 °C, final temperature = 32.2 °C. In this case:

m = grams of water = 50.0 g

c = specific heat of water = 4.18 J/g°C

ΔT = 32.2 – 20.2 = 12.0 °C

Heat energy = (50.0 g)(4.18 J/g°C)( 12.0 °C) = 2508 J = 2.51 kJ (3 sig figs)

This is s neutralization reaction:

H+ (aq) + OH- (aq) 🡪 H2O (l)

mol NaOH = (0.0200 L)(2.00 mol/L) = 0.0400 mol NaOH = 0.0400 mol OH-

mol HCl = (0.0300 L)(2.00 mol/L) = 0.0600 mol HCl = 0.0600 H+

So hydroxide is the limiting reagent.

Per mole of hydroxide,

Heat energy = (2.508 kJ)/(0.04000 = 62.7 kJ / mol

The temperature of the surroundings increased, so the sign of ΔH of the system should be negative:

ΔH = -62.7 kJ / mol

Sources of error:

Assumtion that the density of water is 1.00 g/ cm3. With sodium hydroxide and hydrochloric acid dissolved, the real density is different, but since concentrations are low, it does not introduce much experimental error.

It is also assumed that all of the heat went into the liquid (system), and no heat went into the surroundings. This is not true, but it is usually not a large source of error if the reaction doesn’t take too long.

5.3 Hess’s Law

The enthalpy of the reactants, Hreactants and the enthalpy of the products, Hproducts depend on the bonding of the reactants and products… nothing else. So, the ΔHreaction only depends on the initial and final state of the reaction, not how you got from one state to another state. It is called a “state function”.

Practically speaking, if we can find several equations that “add up” to the equation we want, the ΔHreactions will add up to the overall ΔH. This is called Hess’s Law.

The following example is taken from (and you can find more helpful examples here) <http://www.saskschools.ca/curr_content/chem30/modules/module3/lesson5/hessmore.html>

1) **Calculate the heat released by the burning of sulfur in oxygen given the following steps**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| 2S(s) | + | 3O2 (g) | http://www.saskschools.ca/curr_content/chem30/images/arrow.gif | 2SO3(g) | http://www.saskschools.ca/curr_content/chem30/images/delta.gifH = ? |

**Given Steps**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Step 1 | S(s) | + | O2 (g) | http://www.saskschools.ca/curr_content/chem30/images/arrow.gif | SO2 (g) | http://www.saskschools.ca/curr_content/chem30/images/delta.gifH= | -297 kJ |
| Step 2 | 2SO2 (g) | + | O2 (g) | http://www.saskschools.ca/curr_content/chem30/images/arrow.gif | 2SO3 (g) | http://www.saskschools.ca/curr_content/chem30/images/delta.gifH= | - 198 kJ |

**Answer:**

1) The overall reaction is written above.

Note that sulfur (S) is a reactant and sulfur trioxide (SO3) is the product. Therefore neither reaction in steps 1 or 2 needs to be reversed.   
Note that the overall equation has 2 moles of S and 2 moles of SO3. Therefore the first reaction must be multiplied by two , but the second can be left alone.

2) Manipulate equations

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Step 1 | 2 S(s) | + | 2O2 (g) | http://www.saskschools.ca/curr_content/chem30/images/arrow.gif | **2SO2 (g)** | http://www.saskschools.ca/curr_content/chem30/images/delta.gifH = - 594 kJ |
| Step 2 | 2 SO2(g) | + | O2 (g) | http://www.saskschools.ca/curr_content/chem30/images/arrow.gif | **2 SO3 (g)** | http://www.saskschools.ca/curr_content/chem30/images/delta.gifH = - 198 kJ |

Notice that the SO2 created in step 1 is a reactant in step 2. Substances in bold above will be products

3) Add equations and heats

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Addition: | 2S (s) | + | 3O2 (g) | + | **2SO2 (g)** | http://www.saskschools.ca/curr_content/chem30/images/arrow.gif | **2SO2 (g)** | + | 2SO3 (g) | http://www.saskschools.ca/curr_content/chem30/images/delta.gifH = - 792 kJ |

Substances in bold above are common and are therefore canceled

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Net | 2S (s) | + | 3O2 (g) | http://www.saskschools.ca/curr_content/chem30/images/arrow.gif | 2 SO3 (g) | http://www.saskschools.ca/curr_content/chem30/images/delta.gifH = - 792 kJ |

If you reverse an equation, you must change the sign of http://www.saskschools.ca/curr_content/chem30/images/delta.gifH. (negative becomes positive, positive becomes negative).

**3) Calculate the heat of reaction for the following equation**

C3H8 (g) + 5 O2 (g) -----> 3 CO2 (g) + 4 H2O(g)

given the following steps in the reaction mechanism.

Step #1: 3C (s)+ 4 H2 (g) -------> C3H8 (g)   
Step #2: 2 H2(g) + O2 (g) -------> 2H2O (g)  
Step #3: C (s) + O2 (g) --------> CO2 (g)

**Answer**

1) Overall balanced equation is written above. Note that C3H8 is a reactant and there are 3 moles of CO2 and 4 moles of H2O as products.

2) We can manipulate the equations by:

a) Reversing equation #1  
b) Multiplying equation #2 by 2  
c) Multiplying equation #3 by 3

manipulated equations we get

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Manipulated equations | | | | | | http://www.saskschools.ca/curr_content/chem30/images/delta.gifH |
|  | C3H8 (g) | http://www.saskschools.ca/curr_content/chem30/images/arrow.gif | **4 H2 (g)** | + | **3C (s)** | +103.8 kJ |
|  | 4 H2 (g) | + | 2 O2 (g) | http://www.saskschools.ca/curr_content/chem30/images/arrow.gif | **4 H2O (g)** | -968 kJ |
|  | 3 C (s) | + | 3 O2 (g) | http://www.saskschools.ca/curr_content/chem30/images/arrow.gif | **3 CO2 (g)** | -1180.5 kJ |

the substances in bold print are products

3) Adding the equations we get

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| C3H8 (g) | + | 5O2 (g) | + | **4 H2 (g)** | + | **3 C(s)** | http://www.saskschools.ca/curr_content/chem30/images/arrow.gif | **3 C (s)** | + | **4 H2 (g)** | + | 4 H2O (g) | + | 3 CO2 (g) |

|  |
| --- |
| http://www.saskschools.ca/curr_content/chem30/images/delta.gifH = - 2044.7 kJ |

the substances in bold print are common substances and are canceled to produce the net equation

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| C3H8 (g) | + | 5O2 (g) | http://www.saskschools.ca/curr_content/chem30/images/arrow.gif | 4 H2O (g) | + | 3 CO2 (g) |  | http://www.saskschools.ca/curr_content/chem30/images/delta.gifH = - 2044.7 kJ |

5.4 Bond Enthalpies

5.4.1 **Average bond enthalpy** .Average enthalpy change per mole when the same type of bond is broken in the gas phase for many similar substances

The average bond enthalpy of a C-H bond could be calculated like this:

CH4(g) 🡪 C(g) + 4H(g)

The enthalpy change for this reaction is +1646 kJ mol-1 , so the **average** bond enthalpy is +1646 / 4 = +412 kJ mol-1 . They can be looked up in data tables.

Important: notice two things about the above reaction of methane (CH4). 1. All chemicals are in the gas phase and 2. the products are atoms.

5.4. The enthalpy of a reaction can be calculated from individual bond energies. You can find out how much energy (enthalpy) is needed to break a bond and how much energy you receive when the new bonds are made.

ΔHΘ = Σ BEbonds broken – Σ BEbonds made

The following example is taken from <http://www.kentchemistry.com/links/Kinetics/BondEnergy.htm>

EXAMPLE: Findhttp://www.kentchemistry.com/images/links/Kinetics/delta.gifHhttp://www.kentchemistry.com/images/links/Kinetics/degrees.gif for the following reaction given the following bond energies:  
http://www.kentchemistry.com/images/links/Kinetics/be1a.gif

|  |  |
| --- | --- |
| **Bond** | **Bond Energy** **(kJ/mol)** |
| H-H | 436 |
| O=O | 499 |
| O-H | 463 |

We have to figure out which bonds are broken and which bonds are formed.

2 H-H bonds are broken.

1 O=O bond is broken

2 O-H bonds are formed per water molecule, and there are 2 water molecules formed, therefore 4 O-H bonds are formed

Now we can substitute the values given into the equation:

