Thermochemistry

Thermochemistry is the study of the energy and heat associated with chemical reactions and/or physical transformations.

First law of thermodynamics: Energy cannot be created or destroyed.

Hess law of constant heat summation: The change in enthalpy, that is, the change in heat at constant pressure for any chemical reaction is constant regardless if the chemical reaction occurs in one step or several steps.

1)Calculating heat of reaction using other reactions:

1) Calculate the value of ΔH_{rxn} for the reaction:

$3\ Fe\ (s) + 4\ H_2O(g) \rightarrow Fe_3O_4(s) + 4\ H_2\ (g)$

Given:

$FeO\ (s) + H_2\ (g) \rightarrow Fe(s) + H_2O(g)$ $\quad \Delta H = +24.7$ kj

$3\ FeO\ (s) + \frac{1}{2}\ O_2\ (g) \rightarrow Fe_3O_4\ (s)$ $\quad \Delta H = -317.6$ kj

$H_2\ (g) + \frac{1}{2}\ O_2\ (g) \rightarrow H_2O\ (g)$ $\quad \Delta H = -241.8$ kj

2) Calculate the value of ΔH_{rxn} for the reaction:

$2N_2\ (g) + 5\ O_2\ (g) \rightarrow 2N_2O_5(g)$

Given the following data:

$H_2\ (g) + \frac{1}{2}\ O_2\ (g) \rightarrow H_2O(l)$ $\quad \Delta H = -285.8$ kj

$N_2O_5(g) + H_2O(l) \rightarrow 2\ HNO_3(l)$ $\quad \Delta H = -76.6$ kj

$\frac{1}{2}\ N_2\ (g) + \frac{3}{2}\ O_2\ (g) + \frac{1}{2}\ H_2\ (g) \rightarrow HNO_3(l)$ $\quad \Delta H = -174.1$ kj

2)Calculating heat of reaction using standard heat of formation, $\Delta H°_f$:

The standard heat of formation of a compound, $\Delta H_f°$, is the change in enthalpy for the reaction in which one mole of the compound in its standard state is formed from its elements in their standard states.

For example, ***C(s) + H_2 (g) → CH_4 (g)*** $\Delta H_f° = -74.9$ kj/mole

The above elements are in their standard states.

$\Delta H_f°$ are important since they can be used to calculate heats of reaction that are not conveniently measured directly

Example 1: For the reaction: ***Fe_2O_3 (s) + 3 CO(g) → 2 Fe (s) + 3 CO_2 (g)*** , the value of ΔH_{rxn} is -23.5 kj.

The standard heat of formation of: CO(g) is -110.5 kj/mole

CO_2 (g) is – 393.5 kj/mole

Calculate the standard heat of formation of Fe_2O_3(s).

Example 2: Given the following data for the reaction:

$CH_4(g) + 2\ O_2\ (g) \rightarrow CO_2\ (g) + 2\ H_2O\ (l)$ ΔH_{rxn} is -890.4 kj.

$\Delta H_f°$ for CH_4 (g) = - 74.9 kj/mole

$\Delta H_f°$ for H_2O (l) = - 285.9 kj/mole

Calculate $\Delta H_f°$ for CO_2 (g).

Recall, the standard heat of formation of an element is zero.

3)Calculating heat of reaction using bond energies:

Example1 :Use the average bond energy table to calculate the heat of reaction for the following reaction in the vapor state.

$CH_4(g) + 4\ Cl_2(g) \rightarrow CCl_4(g) + 4\ HCl(g)$

bond	Bond energy	Bond	Bond energy
C-H	414 kj/mole	C-Cl	326 kj/mole
Cl-Cl	243 kj/mole	H-Cl	431 kj/mole

Example2: Use the average bond energy table provided to calculate the heat of reaction for the following:

$N_2(g) + 2\ H_2(g) \rightarrow N_2H_4(g)$

Bond	Bond energy	Bond	Bond energy
N-N triple bond	941 kj/mole	N-H	389 kj/mole
H-H	435 kj/mole	N-N single bond	159 kj/mole

Example3 :Use the average bond energy table to calculate the heat of reaction for the following reaction in the vapor state.

$4\ NH_3\ (g)\ +\ 3\ O_2\ (g) \rightarrow\ 2\ N_2\ (g)\ +\ 6\ H_2O\ (g)$

Bond	Bond energy	Bond	Bond energy
N-H	389 kj/mole	N-N triple bond	941 kj/mole
O-O double bond	494 kj/mole	O-H	464 kj/mole

Example 4 :Use the average bond energy table to calculate the heat of reaction for the following reaction in the vapor state.

$CH_3Cl\ (g)\ +\ \ F_2\ (g) \rightarrow\ CH_2FCl\ (g)\ +\ \ HF\ (g)$

Bond	Bond energy	Bond	Bond energy
C-H	414 kj/mole	C-F	485 kj/mole
F-F	155 kj/mole	H-F	565 kj/mole

Calculating the Amount of Heat Energy Involved in a Chemical Reaction

Specific heat is the amount of heat required to increase the temperature of 1 gram of a substance by 1 ºC

$$\text{Specific heat} = \frac{\text{amount of heat}}{\text{mass} \times \Delta T}$$

The specific heat of water is 4.184 joule/g. ºC

Amount of heat involved in a chemical reaction = Specific heat x mass x ΔT

Exercise: The reaction given below is exothermic

$$Mg\ (s) + 2\ HCl\ (aq) \rightarrow MgCl_2\ (aq) + H_2\ (g)$$

To determine the enthalpy change for the above reaction, 0.158 g of Mg (s) is reacted with excess HCl(aq) to make 100.0 ml solution in a coffee-cup calorimeter.
(A calorimeter is a sealed device that prevents heat from escaping to the outside environment. Also, it prevents external heat from coming in).
The temperature of the solution rises from 23.7 ºC to 30.9 ºC due to the heat produced from the reaction. The density of the solution is 1.00 g/ml and its specific heat is 4.18 J/g ºC . Find ΔH_{rxn} for the reaction as written above.

(Answer: -4.6×10^5 J/mole Mg)

Setup:

Answer_____