Thermodynamics Unit - Enthalpy

1. Calculate the heat evolved from a reaction mixture of 13.4L SO_2 at 1 atm and 273K and 15 g of O_2 .

$$2 SO_2 (g) + O_2 (g) \rightarrow 2 SO_3 (g) \Delta H^{\circ} = -198kJ$$

This is a limiting reagent problem. So we first need to calculate the moles of each reactant:

$$n_{O_2} = \frac{15g}{32 \frac{g}{mol}} = 0.469 moles$$

$$n_{SO_2} = \frac{PV}{RT} = \frac{(1atm)(13.4L)}{(0.08206 \frac{L \bullet atm}{mol K})(273K)} = 0.598 moles$$

Now we divide the number of moles by the species' stoichiometric coefficient:

$$\frac{n_{O_2}}{1} > \frac{n_{SO_2}}{2}$$

$$\frac{0.469mol}{1} > \frac{0.598mol}{2}$$

$$0.469 > 0.299$$

So SO_2 is the limiting reactant. It will dictate how far the reaction can proceed. Now we can actually calculate the ΔH of this particular situation. The value ΔH° refers to exactly 1 mol of O_2 reacting with 2 mol of SO_2 . So, now we have to scale this ΔH° to our reaction, which only has 0.598 mol of SO_2 . $\Delta H = n\Delta H^\circ$

$$\Delta H = (0.598 molSO_2)(\frac{1 molrxn}{2 molSO_2})(-\frac{198 kJ}{1 molrxn})$$

$$\Delta H = -59.202 kJ$$

2. The oxidation of nitrogen in the hot exhaust of jet engines and automobile engines occurs by the reaction

$$N_2(g) + O_2(g) \rightarrow 2 \text{ NO } (g) \Delta H^{\circ} = +180.6 \text{ kJ}$$

a. How much heat is absorbed by the formation of 1.55 mol of NO?

The given ΔH° value is the standard heat of formation that corresponds to 1 mole reaction, which forms 2 moles of NO according to the written chemical equation. So again, we have to tailor the given information to our reality which is 1.55 mol of NO.

$$\begin{split} \Delta H &= n\Delta H^{\circ} \\ \Delta H &= (1.55 mol NO)(\frac{1 mol rxn}{2 mol NO})(\frac{180.6 kJ}{1 mol rxn}) \\ \Delta H &= 139.97 kJ \end{split}$$

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b. How much heat is absorbed by the reaction of 5.45 L of nitrogen measured at 1.00 atm and 273K? (R=0.08206 L*atm*mol^{-1*}K⁻¹)

First we need to determine how many moles of N_2 are present in this situation in order to carry out an analysis similar to part a.

$$\begin{split} n &= \frac{PV}{RT} \\ n &= \frac{(1atm)(5.45L)}{(0.08206\frac{L \bullet atm}{molK})(273K)} \\ n &= 0.243mol \\ \Delta H &= n\Delta H^{\circ} \\ \Delta H &= (0.243molN_{2})(\frac{1molrxn}{1molN_{2}})(\frac{180.6kJ}{1molrxn}) \\ \Delta H &= 43.9kJ \end{split}$$

3. Estimate the heat released when ethene ($CH_2=CH_2$) reacts with HBr to give CH_3CH_2Br . Bond enthalpies are C-H: 412 kJ/mol, C-C: 348 kJ/mol, C=C: 612 kJ/mol, C-Br: 276 kJ/mol, Br-Br: 193kJ/mol, H-Br: 366 kJ/mol.

First draw out the reactants and products to analyze the bond types. Reactants:

$$C=C$$

: Br —— H

4 C-H bonds

1 C=C bond

1 H-Br bond

Products:

5 C-H bonds

1 C-C bond

1 C-Br bond

Work:

$$\begin{split} \Delta H &= \sum nBE_{react} - \sum nBE_{prod} \\ \Delta H &= \left[4(412\frac{kJ}{mol}) + 1(612\frac{kJ}{mol}) + 1(366\frac{kJ}{mol}) \right] - \left[5(412\frac{kJ}{mol}) + 1(348\frac{kJ}{mol}) + 1(276\frac{kJ}{mol}) \right] \\ \Delta H &= -58\frac{kJ}{mol} \end{split}$$

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4. Calculate the standard reaction enthalpy for the reaction of calcite with hydrochloric acid: $CaCO_3(s) + 2HCl(aq) \rightarrow CaCl_2(aq) + H_2O(l) + CO_2(g)$. The standard enthalpies of formation for $CaCO_3(s)$: -1206.9 kJ/mol, $CaCl_2(aq)$: -877.1 kJ/mol, HCl(aq): -167.16 kJ/mol, $H_2O(l)$: -285.83 kJ/mol, $CO_2(g)$: -393.51 kJ/mol.

Work:

$$\begin{split} \Delta H &= \sum n \Delta_f H_{prod} - \sum n \Delta_f H_{react} \\ \Delta H &= \left[1 (-877.1 \frac{kJ}{mol}) + 1 (-285.83 \frac{kJ}{mol}) + 1 (-393.51 \frac{kJ}{mol}) \right] - \left[1 (-1206.9 \frac{kJ}{mol}) + 2 (-167.16 \frac{kJ}{mol}) \right] \\ \Delta H &= -15.22 \frac{kJ}{mol} \end{split}$$

- 5. Which of the following reactions is an enthalpy of formation reaction?
- a. $CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$ (No-CH₄ is NOT an element)
- **b.** $2Fe(s) + 3/2O_2(g) \rightarrow Fe_2O_3(s)$ (Yes-Both reactants are elements in their standard states!)
- c. $C_{diamond}(s) + 2H_2(g) \rightarrow CH_4(g)$ (No-C in its standard state is $C_{graphite}$)
- d. $Hg(s) + \frac{1}{2}O_2(g) \rightarrow HgO(s)$ (No-Hg in its standard state is Hg (1))
- 6. Calculate the change in enthalpy for the combustion of graphite by first stating the combustion reaction and then using the data below.

$$H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(l); \Delta H = -285.83 \text{ kJ/mol}$$

 $CO_2(g) + 2H_2O(l) \rightarrow CH_4(g) + 2O_2(g); \Delta H = 882.00 \text{ kJ/mol}$
 $C_{graphite}(s) + 2H_2(g) \rightarrow CH_4(g); \Delta H = -74. \text{ kJ/mol}$

General Combustion Reaction of Hydrocarbons:

_Fuel (hydrocarbon) +
$$_O_2$$
 (g) \rightarrow $_CO_2$ (g) + $_H_2O$ (l)

Combustion Reaction of Graphite:

$$C_{\text{graphite}}$$
 (s) + O_2 (g) \rightarrow CO_2 (g)

There is no water on products side because there are no hydrogens in the reactants.

Rxn 1 – Flipped and x2: $2H_2O(1) \rightarrow 2H_2(g) + 1O_2(g)$; $\Delta H = +571.66$ kJ/mol

Rxn 2 – Flipped: $CH_4(g) + 2^{1}O_2(g) \rightarrow CO_2(g) + 2H_2O(1)$; $\Delta H = -882.00 \text{ kJ/mol}$

Rxn 3 – Same: $C_{graphite}(s) + \frac{2H_2(g)}{2H_2(g)} \rightarrow \frac{CH_4(g)}{2H_2(g)}$; $\Delta H = -74 \text{ kJ/mol}$

OVERALL:
$$C_{\text{graphite}}(s) + O_2(g) \Rightarrow CO_2(g); \Delta H = -384.34 \text{ kJ/mol}$$

7. Which of $O_2(g)$, $O_2(l)$, $H_2(g)$, $H_2(l)$, $H_2O(g)$, $H_2O(l)$ have a heat of formation equal to zero?

 $O_2(g)$ and $H_2(g)$ because these are both in their elemental form under standard conditions.

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8. Calculate the reaction enthalpy for the formation of anhydrous aluminum chloride by first stating the formation reaction and then using the data below:

2Al(s) + 6HCl(aq) \rightarrow 2AlCl₃(aq) + 3H₂(g); Δ H = -149 kJ/mol HCl(g) \rightarrow HCl(l); Δ H = -74 kJ/mol

 $H_2(g) + Cl_2(g) \rightarrow 2HCl(g); \Delta H = -185 \text{ kJ/mol}$

 $AlCl_3(s) \rightarrow AlCl_3(aq); \Delta H = -323 \text{ kJ/mol}$

A few things to remember about formation reactions:

- Formation reactions only have elements in their standard form as reactants
- The product is the desired compound being formed

Anhydrous aluminum chloride's formula is $AlCl_3$ (s). Also, we will treat HCl (aq) as synonymous to HCl (l).

Chemical Reaction:

Al (s) + (3/2)Cl₂ (g) \rightarrow AlCl₃ (s) OR 2Al (s) + 3Cl₂ (g) \rightarrow 2AlCl₃ (s)

Rxn1 – Same: $2Al(s) + \frac{6HCl(aq)}{2AlCl_3(aq)} + \frac{3H_2(g)}{2AlCl_3(aq)} + \frac{3H_2(g)}{2AlCl_3($

Rxn 2 – X6: $\frac{6HCl(g)}{2} \rightarrow \frac{6HCl(l)}{2}$; $\Delta H = -444 \text{ kJ/mol}$

Rxn 3 – X3: $3H_2(g) + 3Cl_2(g) \rightarrow 6HCl(g)$; $\Delta H = -555 \text{ kJ/mol}$

Rxn 4 – Flipped and x2: $\frac{2AlCl_3(aq)}{2}$ \rightarrow 2AlCl₃(s); $\Delta H = 646$ kJ/mol

OVERALL: $2Al(s) + 3Cl_2(g) \rightarrow 2AlCl_3(s); \Delta H = -502 \text{ kJ/mol}$