Unit 3, Lesson 07: Calculating ΔH using Standard Enthalpies of Formation (ΔH^{o}_{f})

 $\Delta \mathbf{H}$ for a chemical reaction can be measured or calculated using:

- 1. Calorimetry data for chemical reactions
- at constant pressure: $-\Delta H = Q = m \cdot c \cdot \Delta T$
- 2. **Hess's Law** when you know ΔH values for other chemical reactions that can be added to give you your target chemical reaction

3. Standard Molar Enthalpies of Formation (ΔH^{o}_{f})

- defined as the amount of energy released or absorbed when one mole of a compound is formed directly from its elements, in their standard states at SATP (25°C and 100 kPa)
- a) formation equations and their ΔH^{o}_{f} values can be used in Hess's Law or
- b) ΔH^{o}_{f} values can be used mathematically to calculate ΔH

eg. from lab #4: $H_2(g) + \frac{1}{2} O_2(g) \rightarrow H_2O(l)$ $\Delta H^o_f = -285.5 \text{ kJ/mol}$

Writing Formation Equations

• the standard state for an element is its most stable or common form at SATP

For metals: the standard state is defined as neutral atoms eg. Mg (s), Al (s), Zn (s), Hg (l)

For non-metals:

- a) Noble gases are present as neutral atoms in the gas state eg. Ne (g), He (g), Ar (g)
- b) "HOBrFINCI" elements: these elements are found as diatomic molecules at SATP. Their state is indicated on the Periodic Table eg. H₂(g), O₂(g), Br₂(l), F₂(g), I₂(s), N₂(g), and Cl₂(g)
- c) allotropes are non-metals that come in more than one form at SATP
 - i) carbon can be found in its pure state as graphite, diamond, buckminsterfullerene (buckyballs), or even carbon nanotubes. The standard state of carbon is defined as graphite at SATP



- ii) oxygen can be found in its pure state as oxygen gas $O_2(g)$ or ozone $O_3(g)$. The standard state of oxygen is defined as oxygen gas, $O_2(g)$ at SATP
- iii) sulfur can be found as S (rhombic sulfur) or S_8 (s). The standard state is rhombic S (s) at SATP
- iv) phosphorus can be P (s) or P_4 (s). P_4 (s) is defined as the standard state of phosphorus at SATP

The standard enthalpy of formation (ΔH°_{f}) of elements in their standard state is zero, by definition.

2 Cl (g)	\rightarrow	$Cl_{2}(g)$	$\Delta H^{\circ}_{f} = 0.00 \text{ kJ/mol}$	(By definition, these reactions require
2 O (g)	\rightarrow	$O_{2}(g)$	$\Delta H^{o}_{f} = 0.00 \text{ kJ/mol}$	and release no energy)

Formation equations for compounds:

Chemists have carefully measured "Standard Molar Enthalpies of Formation" (ΔH^{o}_{f}) for many common substances (p. 597). These can be used, along with Hess's Law, to calculate enthalpies of reaction, ΔH . When you write formation equations, pay attention to the state of the substances and you may need to use fractional coefficients in your formation equations.

eg. Write the formation equations for these different compounds:

testosterone, C₁₉H₂₈O₂:

 $19 C(s) + O_2(g) + 14 H_2(g) \rightarrow C_{19}H_{28}O_2(s)$

eg. aluminum hydroxide, Al(OH)₃:

Al (s) + + 3/2 O₂ (g) + 3/2 H₂ (g) \rightarrow Al(OH)₃ (s)

eg. guanine, from DNA, $C_5H_5N_5O$

 $5 C (s) + \frac{1}{2} O_2 (g) + \frac{5}{2} H_2 (g) + \frac{5}{2} N_2 (g) \rightarrow C_5 H_5 N_5 O (s)$

a) Using standard enthalpies of formation with Hess's Law

(you can recognize this type of problem because you are only given one reaction and its ΔH value)

eg. The complete combustion of glucose $C_6H_{12}O_6$ (s) produces 2805 kJ of energy per mole of glucose burned. Calculate the heat of formation of glucose.

Step 1: Write the target equation and the equation for the combustion of glucose.

We want to calculate the heat of formation of glucose, so our **target equation** will be:

 $6 \ C \ (s) \ + \ 3 \ O_2 \ (g) \ + \ 6 \ H_2 \ (g) \ \longrightarrow C_6 H_{12} O_6 \ (s) \ \Delta H^o{}_f \ = \ ?$

Given: ΔH°_{rxn} for the combustion of one mole of glucose (heat is produced, so ΔH is negative):

$$C_6H_{12}O_6(s) + 6 O_2(g) \rightarrow 6 CO_2(g) + 6 H_2O(g) \Delta H^{\circ}_{rxn} = -2805 \text{ kJ/mol}$$

Step 2: Write the combustion equation for glucose, but flip it to get glucose as a product (like it is in the target equation). Remember to reverse the sign for ΔH° when you flip an equation:

$$6 \text{ CO}_2(g) + 6 \text{ H}_2\text{O}(g) \rightarrow \text{C}_6\text{H}_{12}\text{O}_6(s) + 6 \text{ O}_2(g) \qquad \Delta \text{H}^\circ_{\text{rxn}} = +2805 \text{ kJ/mol}$$

Step 3: To get to the target reaction, we need to eliminate the CO₂ and H₂O. We haven't been given equations with these substances, so we have to use formation reactions. Write the formation equations (pay attention to states) and look up the ΔH°_{f} on page 597.

$$C(s) + O_2(g) \rightarrow CO_2(g) \qquad \Delta H^o_f = -393.5 \text{ kJ/mol}$$

$$H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(g) \qquad \Delta H^o_f = -241.8 \text{ kJ/mol}$$

Step 4: Using Hess's Law, rearrange the given equation and formation equations to give the target equation. Put reactants and products on the correct side of the equation for the target reaction, and multiply the ΔH^{o}_{f} values as necessary:

$6 CO_2(g) + 6 H_2O(g)$	$\rightarrow C_6 H_{12} O_6 (s) + 6 O_2 (g)$	$\Delta H^{\circ}_{rxn} = +2805 \text{ kJ/mol}$
$6 C(s) + 6 O_2(g)$	$\rightarrow 6 \mathscr{E} O_2(g)$	$\Delta H^{o}_{f} = 6 \text{ x} (-393.5 \text{ kJ/mol})$
$6 H_2(g) + 3 O_2(g)$	\rightarrow 6 $H_2O(g)$	$\Delta H^{o}_{f} = 6 \text{ x} (-241.8 \text{ kJ/mol})$

 $6 C (s) + 3 O_2 (g) + 6 H_2 (g) \rightarrow C_6 H_{12} O_6 (s) \qquad \Delta H^o_f = -1006.8 \text{ kJ/mol}$

Using ΔH^{o}_{f} Values to Calculate ΔH Mathematically

If we know the ΔH^{o}_{f} for all of the products and reactants in a chemical reaction, we can take a mathematical short cut to find ΔH^{o} .

The change in enthalpy for a reaction is equal to the overall sum of the standard enthalpies of formation of the products minus the overall sum of the standard enthalpies of formation of the reactants.



eg. Calculate the overall enthalpy change for the combustion of liquid benzene (C_6H_6) in oxygen:

Step 1: Write the target reaction:

 $C_6H_6(l)$ + 15/2 $O_2(g)$ \rightarrow 6 $CO_2(g)$ + 3 $H_2O(g)$ ΔH^o_{rxn} = ?

Step 2: Because we can look up the ΔH°_{f} values for all reactants and products on page 597, we can use the mathematical short cut above. Use the ΔH°_{f} values on page 597 of McGraw-Hill.

$$\Delta H^{o}_{rxn} = \sum (n \Delta H^{o}_{f} \text{ products}) - \sum (n \Delta H^{o}_{f} \text{ reactants})$$

$$= \sum [(6 \times \Delta H^{o}_{f} \text{ CO}_{2(g)}) + (3 \times \Delta H^{o}_{f} \text{ H}_{2} \text{ O}_{(g)})] - \sum [(\Delta H^{o}_{f} \text{ C}_{6} \text{ H}_{6(l)}) + (15/2 \Delta H^{o}_{f} \text{ O}_{2(g)})]$$

$$= \sum [(6 \times -393.5 \text{ kJ}) + (3 \times -241.8 \text{ kJ})] - \sum [(+49.1 \text{ kJ})] + (15/2 \times 0 \text{ kJ})]$$

$$= \sum [-2361 \text{ kJ} + (-725.4 \text{ kJ})] - \sum [49.1 \text{ kJ} + 0 \text{ kJ}]]$$

$$= -3086.4 \text{ kJ} - 49.1 \text{ kJ}$$

$$= 3135.5 \text{ kJ} \text{ of heat released when one mole of } C_{6} \text{ H}_{6} \text{ is burned}$$

eg. Calculate the enthalpy of reaction ΔH^{o}_{rxn} for the following reaction:

$$CS_{2}(g) + 2 H_{2}O(l) \rightarrow CO_{2}(g) + 2 H_{2}S(g) \qquad \Delta H^{o}_{rxn} = ?$$

$$\Delta H^{o}_{rxn} = \sum(n \Delta H^{o}_{f} \text{ products}) - \sum(n \Delta H^{o}_{f} \text{ reactants})$$

$$= \sum[(\Delta H^{o}_{f} CO_{2(g)}) + (2 x \Delta H^{o}_{f} H_{2}S_{(g)})] - \sum[(\Delta H^{o}_{f} CS_{2(g)}) + (2 \Delta H^{o}_{f} H_{2}O_{(l)})]$$

$$= \sum[(-393.5 \text{ kJ}) + (2 x (-20.6 \text{ kJ})] - \sum[(+116.7 \text{ kJ}) + (2 x -285.8 \text{ kJ})]$$

$$= -435.1 \text{ kJ} - (-454.9 \text{ kJ})$$

$$= +19.8 \text{ kJ}$$
Careful of the signs!!

Summary: Δ H can be measured or calculated many ways:

- 1. Experimentally using calorimetry
- 2. Using Hess's Law if you are given all of the needed chemical equations
- 3. Using Hess's Law and standard enthalpies of formation if you are given only one of the needed chemical equations
- 4. Mathematically using the equation $\Delta H^{o}_{rxn} = \sum (n \Delta H^{o}_{f} \text{ products}) \sum (n \Delta H^{o}_{f} \text{ reactants})$ when you can look up the standard enthalpies of all reactants and products

Homework:

- 1. Read pages 250 to 253
- 2. Do questions 17-20 on page 251 of McGraw-Hill
- 3. Do questions 21 to 24 on page 254 of McGraw-Hill (for questions 21 and 22, they do not ask you to find the ΔH° , they just want you to rearrange the equations to arrive at the target equation).
- 4. Do questions 3,4,5 on page 255
- 5. Do question 8 on page 262