

Thermochemistry to date

It's simply about tracking energy(usually in the form of heat)changes that accompany a change of state.

$$\Delta E=q+w$$

- $q=C_s * m * \Delta T$; $q=C_p * \Delta T$ and $q=C_n * n * \Delta T$
note:specific heats of the elements are on your P Table.
- $(C_s * m * (T_2 - T_1))_{\text{sample 1}} = - (C_s * m * (T_2 - T_1))_{\text{sample 2}}$
there will be variations using Cp and Cn.
- q_v, q_p and enthalpy, ΔH
- **The thermochemical equation-stoichiometry of heat**
- **Hess' Law and its applications**
 - manipulating and combining thermochemical equations
 - Born-Haber cycles
 - $\Delta H = \sum \Delta H_f(\text{products}) - \sum \Delta H_f(\text{reactants})$
 - $\Delta H = \sum \text{Bonds broken} - \sum \text{Bonds formed}$

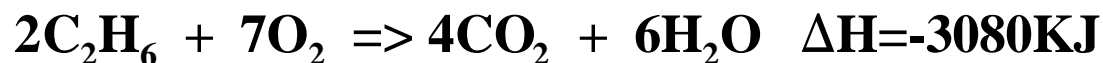
Problems in Thermochemistry

- **Problems involving $\Delta E = q + w$ or simple heat and temperature changes are considered basic and will not be done in class. However, students who encounter difficulties in these areas should seek help immediately.**
- **Heat transfer (the horseshoe revisited)- The problem must begin with careful identification of the data and its appropriate entry into the general heat transfer equation. An error at this point dooms the process**
 - $q_l = -q_g \quad (C_p \Delta T)_{\text{horseshoe}} = -(C_s m \Delta T)_{\text{water}}$
 - $478 \cdot (T_2 - 640) = -4.184 \cdot 5000 \cdot (T_2 - 25)$
- **The web pages present the solution in terms of the rearranged general equation. Realistically, going directly there is not a viable methodology. Rather, all of the terms should be first evaluated as fully as possible and the algebra then done**
 - $478 \cdot T_2 - 306000 = -20920 \cdot T_2 + 523000$
 - $21398 \cdot T_2 = 829000$
 - $T_2 = 38.7$
 - **In a heat transfer problem where a T is determined, the validity of the result is usually verifiable by evaluating each of the heat terms**
 - $478 \cdot (38.7 - 640) = -28700$
 - $4.184 \cdot 5000 \cdot (38.7 - 25) = 28700$

- 26.7g of water at 16.8° are combined with 72.9g of water at an unknown temperature. The resultant mixture has a temperature of 52.3°. What was the initial temperature of the second sample?
- What is your expectation?
- $q_g = -q_l \quad (C_s * m * \Delta T)_{\text{cold}} = -(C_s * m * \Delta T)_{\text{hot}}$
- $4.184 * 26.7 * (52.3 - 16.8) = -4.184 * 72.9 * (52.3 - T_1)_{\text{hot}}$
- $3966 = -15950 + 305T_1$
- $19916 = 305T_1$
- $T_1 = 65.3^\circ$ (meet your expectation?)
- q_g was already fully evaluated as 3966J
- $q_l = 4.184 * 72.9 * (52.3 - 65.3) = -3965J$
- The agreement in these two values does not verify the solution. Why? Thus, all critical “preliminary” calcs should be repeated.
- Do not be surprised if there are slight differences between q_l and q_g . Errors in the problem analysis will lead to very large differences between the two.

- **1.4kg of Fe ($C_n=23.7\text{J}/\text{mole-deg}$) at 623°C are dropped into a container of water at 20.0°C . The final temperature was 61.2°C . What was the mass of the water?**
- **can you form any expectation here? (C_n for water is about $75\text{J}/(\text{mol-deg})$ C_s for Fe is about $0.4\text{J}/(\text{g-deg})$)**
- **$1.4\text{kg}=1400\text{g}$**
- **$n=1400\text{g}/55.85\text{g}/\text{mole}=25.1\text{moles}$**
- **$q_l=C_n*n*(61.2-623)=23.7*25.1*-562=-334000\text{ J}$**
- **$q_g=334000\text{J}=4.184*m*(41.2)$**
- **$m=334000/(4.184*41.2)=1940\text{g}$**
- **does this seem reasonable?**

Stoichiometry of Heat



What is the heat of combustion of C_2H_6 ?

Heat of combustion is per mole. The above equation has 2 moles of C_2H_6 , so the heat of combustion is $-3080\text{KJ}/2 = -1540\text{KJ/mole}$

What is the heat for the reaction of 16.7g of O_2 ?

Using standard stoichiometric analysis-all relations are direct.

The stoichiometric mass of O_2 is 224g.

$$(\quad / \quad)^* = \text{KJ}$$

$$(3080/224)*16.7 = -230\text{KJ}.$$

What do you think the most common error here is?

What is the heat for the production of 0.50moles of C_2H_6 ?

Reversing the reaction changes the sign of the enthalpy.

Again, treating this according to standard stoichiometry.

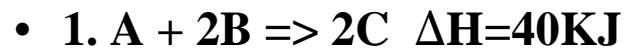
$$(3080/2)*0.50 = 770\text{KJ}$$

Applying Hess' Law

- **The key principle here is that all routes between two states must have the same enthalpy. Thus, the unknown enthalpy for a reaction can be determined by the combination of reactions with known enthalpies.**
 - **The key to an effective approach is finding a unique link between the contributor and the final reaction in terms of a chemical species which is unique to both**
- **In developing the solution, there are only two decisions which need to be made with regards to the contributing reactions:**
 - **the direction in which the contributor is to be written**
 - **the quantity of the contributor which is needed**
 - **these decisions should be made systematically and the effect of each on the contributing heat term noted. A table is often useful in doing this.**

- **Generic first:**

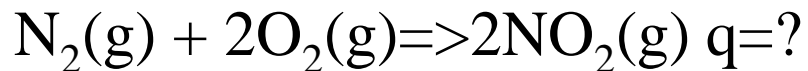
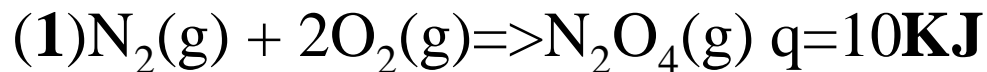
- **given:**



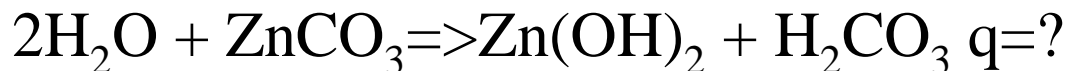
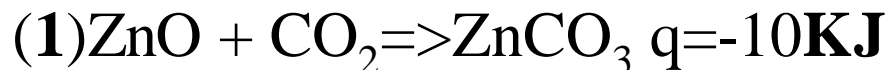
- **what is ΔH for $A + 2D \Rightarrow 2F$?**

Need	Dir	Qty
1. (A)	OK 40	x1 40
2. (F)	Rev 20	x2 40
		80

Use the thermochemical equations shown below to determine the enthalpy for the final reaction:

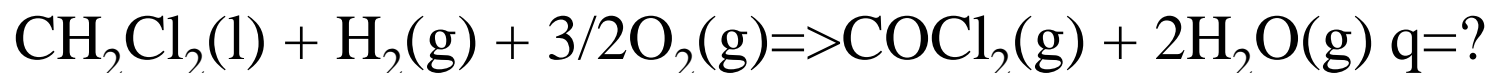
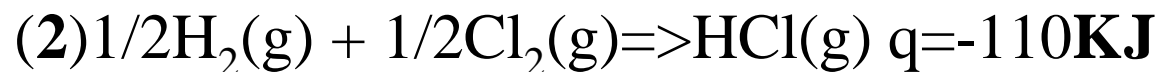


Use the thermochemical equations shown below to determine the enthalpy for the final reaction:



- Use the thermochemical equations shown below to determine

the enthalpy for the final reaction:



Using Heats of Formation

- A new web page (#69) has been added and will be use to present problem analysis in this area.