Chem E-1a **Friday Review Notes Chapter 6: Energy Relationships in Chemical Reactions**

Transfers of Heat and Calorimetry:

For "Calorimetry" Problems:

•This would be any problem that involves mixing different things together, perhaps at different temperatures or with reactions or phase changes occurring, and includes calculations that deal with the initial and final temperatures of the system.

•At the end of the problem, the different components will have reached thermal equilibrium, which means that they will all be at the same temperature.

•Typically (even if it is not explicitly stated!) we will assume that these problems are carried out in a perfectly insulated container, and thus the sum of the q's for each component of the system will add up to zero:

For any standard "calorimetry" problem:

$$q_1 + q_2 + q_3 + \dots = 0$$

where q_1, q_2, q_3 , etc, are the heat transfers involved with each temperature change, phase change, or reaction for each component of the system.

Calculating q:

For Any Substance Changing Temperature:

$q = ms\Delta T$

 \mathbf{q} = heat exchange of the substance changing temperature (typically in J or kJ) \mathbf{m} = mass of the substance changing temperature (typically in units of grams)

 \mathbf{s} = specific heat of the substance (typically in J/g•K or J/g•°C)

 $\Delta \mathbf{T} = \text{change in temperature} = T_{\text{final}} - T_{\text{initial}} \quad (\text{in units of °C or K})$ (Note: Because a *change* in °C is equivalent to a *change* in Kelvin, reporting ΔT is the one instance in which you can switch between °C and K without changing the number at all. For example, a ΔT of 20°C is equivalent to a ΔT of 20 K.)

In some instances you may be given a molar heat capacity (in units of J/mol•K or J/mol•°C) instead of a specific heat. In a case like this you can still use essentially the same formula to calculate q, except you would need to plug in moles of the substance rather than mass in order for the units to cancel out. If you make sure that your units always cancel correctly, you can adjust this formula as needed without the necessity of "memorizing" a variety of different formulas.

For A Bomb Calorimeter Changing Temperature:

$$q = C_{cal} \Delta T$$

 $\begin{array}{l} \mathbf{q} = \text{heat exchange of the bomb calorimeter (typically in J or kJ)} \\ \mathbf{C_{cal}} = \text{heat capacity of the calorimeter (typically in units of kJ/°C or kJ/K)} \\ \boldsymbol{\Delta T} = \text{change in temperature} = T_{\text{final}} - T_{\text{initial}} \quad (\text{typically in units of °C or K)} \end{array}$

For All Reactions, Including Phase Changes:

 $q = n\Delta H$

 \mathbf{q} = heat exchange of the reaction or the phase change (typically in units of J or kJ) \mathbf{n} = number of moles of reaction (in units of moles) (Note: see discussion below about n) ΔH = change in enthalpy of the reaction or the phase change (in units of J/mol or kJ/mol)

A note on "n", which is the number of moles of reaction:

 $n = \frac{number of moles of something that reacts or is produced}{stoichiometric coefficient in the balanced chemical reaction}$

According to this definition, you should notice that if a reaction (such as a phase change reaction or a combustion reaction) has a substance with a coefficient of "1" in front of it, then "n" is simply the number of moles of that substance that changes phase or combusts. Also note that "n" is NOT equal to the sum of the number of moles of everything that reacts. If there is a reaction that goes to completion, "n" is equal to the number of moles of the limiting reagent divided by its stoichiometric coefficient. In addition, if you draw up a RICE table for a reaction, then "n" is equal to "x" in your RICE table.

Some specific ΔH 's:

 ΔH_{fusion} = enthalpy change for 1 mole of a substance changing from (s) \rightarrow (l)

 $\Delta H_{\text{vaporization}} = \text{enthalpy change for 1 mole of a substance changing from } (l) \rightarrow (g)$ $\Delta H_{\text{combustion}} = \text{enthalpy change for the combustion of 1 mole of a substance}$

Energy, Heat, and Work:

 $\Delta U = q + w$

 ΔU = change in Internal Energy of the system (in units of J or kJ) q = heat transferred into the system (in units of J or kJ) (We saw above all the ways to calculate q!) w = work done on the system (in units of J or kJ)

Calculating w:

We can calculate the work done whenever the volume of a system changes against a constant external pressure:

 $w = -P_{ext}\Delta V$

w = work done on the system (in units of either J or kJ or in units of L•atm) P_{ext} = external pressure on the system (in units of atm) ΔV = change in volume of system = $V_{final} - V_{initial}$ (in units of L)

Note the following conversion factor: 1 L•atm = 101.3 J

A Note on Sign Conventions:

It is important to become comfortable with the sign conventions for q, w, ΔH , and ΔU . You should be able to determine the sign (either "+" or "-") of these values if you are given a description of a certain process, even without doing calculations. Then, when you do the calculations, always check to make sure that your answers agree with what you would expect.

A couple important things to remember:

•An **exothermic** reaction gives off heat, and has a negative ΔH ($\Delta H < 0$). If an exothermic reaction occurs, the temperature of the reaction vessel will increase.

•An endothermic reaction absorbs heat, and has a positive ΔH ($\Delta H > 0$). If an endothermic reaction occurs, the temperature of the reaction vessel will decrease.

Hess's Law and Heat of Formation Problems:

You can calculate the ΔH of a reaction from the ΔH 's of other reactions, or by using tabulated values of ΔH°_{f} .

Hess's Law:

•If you reverse the direction of a balanced equation, you switch the sign on ΔH .

•If you double all coefficients in a balanced equation, you multiply ΔH by 2. If you triple the coefficients, you multiply the ΔH by 3, etc. In general, if you multiply all of the coefficients in a reaction by a number, you should multiply the ΔH by that number.

•If you add up two balanced equations and cancel things out, you add up the ΔH 's.

Heats of Formation (ΔH_{f}) :

$\Delta H_{rxn} = \sum m \Delta H_{f}^{\circ}(\text{products}) - \sum m \Delta H_{f}^{\circ}(\text{reactants})$

(Note: "m" represents the stoichiometric coefficients of each particular substance in the balanced chemical reaction.)

 ΔH_f° is the change in enthalpy for the reaction in which one mole of a compound is formed from its elements in their standard states. (Be aware of the standard phases of the elements and of the 7 elements that exist as diatomic molecules.)