Worksheet 2

1. Energy and Enthalpy.
A system can exchange energy with its surroundings either by transferring heat or by doing work. Using q to represent transferred heat and w = - $P\,\Delta V$, the total energy change of a system, ΔU, can be represented as

$$\Delta U = q + w = q - P\,\Delta V$$

where q has a positive sign if the system gains heat and a negative sign if the system loses it. Rearrange this equation to give the amount of heat transferred. Then, think of two ways in which a chemical reaction might be carried out: a reaction might be carried out in a closed container with a constant volume, or carried out in an open flask that keeps the pressure constant and allows the volume of the system to change freely. Write out the two equations that would describe these two scenarios in terms of heat transfer and/or PV work. Lastly, the enthalpy (H) of a system is described by the quantity $U + PV$. What is the equation that relates heat to enthalpy at constant pressure?

2. Fill in the blanks.
When reactions are performed in an open container, such as a coffee-cup calorimeter, the ______ does not change and q_p = ___; in a closed container, such as a bomb calorimeter, the ______ does not change and q_v = ___. Remember that even in an open container, unless a gas is involved in the reaction, volume changes are usually negligible and $\Delta H \cong \Delta U$.

3. What are extensive and intensive properties and some examples of each?

4. Suppose the enthalpy change when carbon monoxide is burned with oxygen to carbon dioxide is given by the reaction

$$\_C(s,gr) + \_\ O_2(g) \rightarrow \_CO(g) \qquad \Delta H = -110.5\ \text{kJ}$$

at 25°C. What is the internal energy of this reaction?

5. Calculate $\Delta H°_f$ (in kilojoules per mole) for benzene, C_6H_6, from the following data:

$$2\ C_6H_6(l) + 15\ O_2(g) \rightarrow 12\ CO_2(g) + 6\ H_2O(l) \qquad \Delta H = -6534\ \text{kJ}$$

$\Delta H°_f$ (CO_2) = -393.5 kJ/mol
$\Delta H°_f$ (H_2O) = -285.8 kJ/mol

6. Use the bond dissociation energies found in the eBook under Data and Tables to calculate an approximate $\Delta H°$ (in kilojoules) for the reaction of ethylene with hydrogen to yield ethane.

$$H_2C{=}CH_2(g) + H_2(g) \rightarrow CH_3CH_3(g)$$

7. In your own words describe what entropy, spontaneity, microstates are in relation to thermodynamics.

8. Predict whether $\Delta S°$ is likely to be positive or negative for each of the following reactions:

(a) $H_2C{=}CH_2(g) + Br_2(g) \rightarrow CH_2BrCH_2Br(l)$
(b) $2\ C_2H_6(g) + 7\ O_2(g) \rightarrow 4\ CO_2(g) + 6\ H_2O(g)$

9. What is the equation for Gibbs free-energy change (ΔG) and what does each quantity define? Remember that the value of the free-energy change ΔG is a general criterion for the spontaneity of a chemical or physical process.

10. The two gases $BF_3(g)$ and $BCl_3(g)$ are mixed in equal molar amounts. All B—F bonds have about the same bond enthalpy, as do all B—Cl bonds. Explain why the mixture tends to react to form $BF_2Cl(g)$ and $BCl_2F(g)$.

11. Tetraphenylgermane, $(C_6H_5)_4Ge$, has a melting point of 232.5°C, and its enthalpy increases by 106.7 J g^{-1} during fusion. Calculate the molar enthalpy of fusion and molar entropy of fusion of tetraphenylgermane.

12. Suppose 1.00 mol of water at 25°C is flash-evaporated by allowing it to fall into an iron crucible maintained at 150°C. Calculate ΔS_{tot}, if $c_p(H_2O(l)) = 75.4$ J K^{-1} mol^{-1} and $c_p(H_2O(g)) = 36.0$ J K^{-1} mol^{-1}. Take $\Delta H_{vap} = 40.68$ kJ mol^{-1} for water at its boiling point of 100°C.

13. Iron has a heat capacity of 25.1 J K^{-1-} mol^{-1}, approximately independent of temperature between 0 and 100°C. Calculate the enthalpy and entropy change of 1.00 mol of iron as it is cooled at atmospheric pressure from 100°C to 0°C.

14. A water bath is filled with lots of ice and water to maintain a constant temperature of 0°C. You dump a 10 g block of 200°C aluminum into the bath. The heat capacity of aluminum is 24.35 J K^{-1} mol^{-1} and the enthalpy of fusion of water is 6 kJ mol^{-1}.

(a) How much heat is transferred from the block to the water bath?
(b) How many grams of ice melt?
(c) What is the entropy change of the aluminum block?
(d) What is the entropy change of the water bath?
(e) What is the total entropy change?

15. The following reaction is performed at a constant temperature of 298 K and a pressure of 1 atm. Given that $\Delta H°_f\ (NH_3)(g) = -46.11$ kJ mol^{-1} and $\Delta G°_f\ (NH_3)(g) = -16.48$ kJ mol^{-1}.

$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$$

If the reaction moves from reactants to products what sign would you expect for each of the following:

q	Positive	Negative	Zero	No Way to Know
w	Positive	Negative	Zero	No Way to Know
ΔH (system)	Positive	Negative	Zero	No Way to Know
ΔS (system)	Positive	Negative	Zero	No Way to Know

Comparing the energy and the enthalpy you would expect which of the following describes this reaction:

$\Delta H > \Delta U$ $\qquad$ $\Delta H < \Delta U$ $\qquad$ $\Delta H = \Delta U$

Do you expect the reaction to be "spontaneous"? Yes No

If "Yes" or "No" is there a temperature at which it will be non-spontaneous/spontaneous?