## Chem 531: Problem Set #3

Due in class: Tues, Sept. 26th

(1) When nitroglycerin explodes, the chemical reaction that occurs can be assumed to be

$$C_{3}H_{5}N_{3}O_{9}(l) \rightarrow 3CO_{2}(g) + \frac{5}{2}H_{2}O(g) + \frac{3}{2}N_{2}(g) + \frac{1}{4}O_{2}(g)$$

- (a) Calculate  $\Delta H_r^o$  and  $\Delta U_r^o$  for this reaction at 298 K, given that the enthalpy of formation of liquid nitroglycerin at 25°C is -372.4 kJ/mol.
- (b) Consider 0.20 mol of nitroglycerin at 25°C completely filling a constant volume cell of 0.030 L. Calculate the *maximum* temperature and pressure that would be generated by the explosion of the nitroglycerin if the constant-volume cell did not burst (or vaporize). You may assume that (1) the explosion occurs so rapidly that the conditions are adiabatic, (2) the pressure cell comes to immediate thermal equilibrium with the products, (3) the products are ideal gases, and (4) the total constant volume heat capacity of products plus cell has the temperature-independent value of 100 J/K.
- (2) Calculate the change in entropy of the system, the surroundings, and the total change in entropy (universe) if one mole of an ideal gas is expanded isothermally and reversibly from a pressure of 10.0 bar to 2.00 bar at 300 K.
- (3) Redo problem #2 for an expansion into a vacuum, with an initial pressure of 10.0 bar and a final pressure of 2.00 bar.
- (4) A 25.0 g mass of ice at 273 K is added to 150.0 g of H<sub>2</sub>O(*l*) at 360 K at constant pressure in an adiabatic container. Is the final state of the system ice or liquid water? Calculate  $\Delta S$  for the process. Is this process spontaneous? (Base your answer on  $\Delta S_{univ}$ )
- (5) 1.00 kg of water at 90°C is dumped into a swimming pool filled with water at 30°C. The swimming pool is effectively isolated from the surroundings and acts as a reservoir at 30°C. Calculate the entropy change of the system (water+pool), the surroundings, and the universe. Take the (specific) heat capacity of water as a constant at 4.18 J g<sup>-1</sup> K<sup>-1</sup>.

(6) One mole of liquid water is supercooled to  $-2.25^{\circ}$ C at 1 bar pressure. Of course the normal freezing temperature of water at this pressure is 0.00°C. The transformation H<sub>2</sub>O(*l*)  $\rightarrow$  H<sub>2</sub>O(s) is suddenly observed to occur. By calculating  $\Delta S$ ,  $\Delta S_{surr}$ , and  $\Delta S_{univ}$ , verify that this transformation is spontaneous at  $-2.25^{\circ}$ C. The heat capacities are given by 75.3 and 37.7 J K<sup>-1</sup> mol<sup>-1</sup> for H<sub>2</sub>O(*l*) and H<sub>2</sub>O(s), respectively.  $\Delta H_{fus}^o = 6.008$  kJ mol<sup>-1</sup> at 0.00°C. Assume that the surroundings are at  $-2.25^{\circ}$ C.