Homework, Week 6

1. Chloroform can be synthesized from natural gas and elemental chlorine according to the following reaction:

$$CH_4(g) + 3\ Cl_2\ (g) \leftrightarrow CHCl_3(l) + 3\ HCl(g)$$
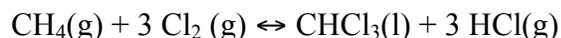
   a) Determine $\Delta G°_{rxn}$ for this system.

   b) Assuming $\Delta H°_f$ and $S°_m$ remain constant, will this reaction proceed spontaneously at 500 K?

   The following data could be useful.

	$CH_4(g)$	$Cl_2(g)$	$CHCl_3(l)$	$HCl(g)$
$\Delta H°_f$ (kJ/mol)	-74.81	0	-135.44	-92.31
$S°_m$ (J/K mol)	186.26	223.07	216.40	186.91
$\Delta G°_f$ (kJ/mol)	-50.72	0	-73.66	-95.30
ρ (g/cm³)	0.720	0.940	1.499	1.187

2. The protein lysozyme unfolds at a transition temperature of 75.5 °C with $\Delta H_{unfold} = 509$ kJ mol⁻¹. Calculate the entropy of unfolding of lysozyme at 25°C, given that the difference in the constant-pressure heat capacities upon unfolding is 6.28 kJ K⁻¹ mol⁻¹ and is assumed to be independent of temperature.

3. The molar enthalpy of vaporization of chloroform ($CHCl_3$) at its normal boiling point, 80.1°C, is 30.7 kJ mol⁻¹. Assuming that ΔH_{vap} and ΔS_{vap} remain constant, determine ΔG_{vap} at 75°C, 80.1°C, and 85°C.

4. Most of the portable red fire extinguishers that you see in public buildings or can purchase for your home (the so-called "ABC dry chemical" extinguishers) contain powdered sodium bicarbonate that decomposes when exposed to high temperature (for example from a fire) into sodium carbonate, water, and carbon dioxide:

$$2\ NaHCO_3(s) \rightarrow Na_2CO_3(s) + H_2O(g) + CO_2(g)$$

a) Determine the equilibrium constant of the reaction at 150°C.

b) At equilibrium, if the partial pressure of $CO_2(g)$ is 0.80 atm, what is the partial pressure of $H_2O(g)$?

5. The water-gas shift reaction is an important industrial source of pure $H_2(g)$ for ammonia synthesis:

$$CO(g) + H_2O(g) \leftrightarrow H_2(g) + CO_2(g)$$
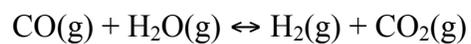
What would happen to the equilibrium concentration of each species if you increase the total pressure of the system by a factor of 100?

6. Under certain conditions, water vapor dissociates into $H_2(g)$ and $O_2(g)$. At 2100 K and 1 bar, the equilibrium constant for the dissociation reaction is twice as large as at 2000 K and 1 bar. Determine the enthalpy of the dissociation reaction, assuming it is constant over this temperature range.