CHEM442-001/002
College of Charleston
Spring 2000
Exam I

1(10). Consider the following two chemical reactions

$$2\ OH(g) \rightarrow H_2O_2(g) \qquad (1)$$
$$2\ OH(g) \rightarrow H_2(g) + O_2(g) \qquad (2)$$

Given $\Delta_f G^o_{298}/(\text{kJ mol}^{-1}) = 34.23$ for OH(g) and -105.57 for H_2O_2(g), calculate $\Delta_r G^o_{298}$ for each reaction.

Which reaction is more spontaneous?

2(10). For the reaction

$$2\ OH(g) \rightarrow OH^-(g) + OH^+(g) \qquad \Delta_r G^o_{298} = 1099.28\ \text{kJ}$$

the value of $\Delta_r H^o_{298} = 1068.10$ kJ and is relatively constant over small temperature intervals. Calculate $\Delta_r G^o_{200}$ for this reaction.

Has the spontaneity of this reaction increased at this lower temperature?

3(10). Beginning with the differential energy expression

$$dG = -S\ dT + V\ dP$$

derive the Maxwell relationship that begins $(\partial S/...)$.

4(20). Consider an infinite universe of atomic hydrogen at 5 K. Calculate $\Delta\epsilon$, the energy difference in J between the $n = 5$ and the $n = 1$ energy levels.

Calculate N_5/N_1, the ratio of the numbers of atoms in the $n = 5$ level compared to the $n = 1$ energy level.

5(30). Given

$$R_{n,l}(r) = -\left[\frac{(2Z/na_o)^3\ (n-l-1)!}{2n[(n+l)!]^3}\right]^{1/2} e^{-\rho/2}\ \rho^l\ L^{2l+1}_{n+l}(\rho)$$

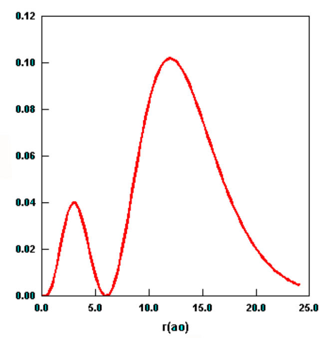
where $\rho = (2Z/na_o)$ and

$$L_q^s(x) = \frac{d^s}{dx^s}\, e^x\, \frac{d^q}{dx^q}\left(x^q\, e^{-x}\right)$$

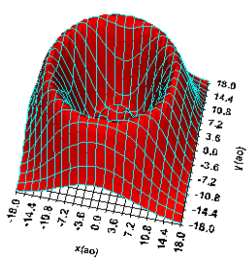
derive the radial wave function for a 2p subshell. You may leave your answer expressed in terms of ρ rather than converting to r.

6(20). The following are screen captures from the P-Chem software.

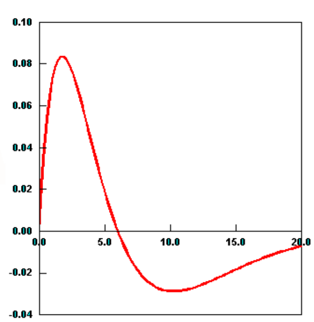
(1)



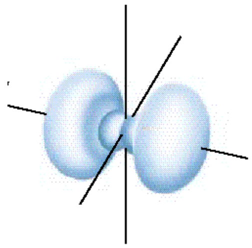
(2)



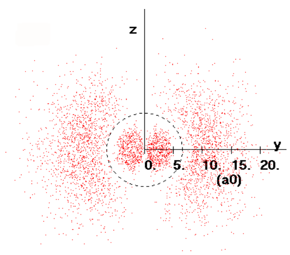
(3)



(4)



(5)



Which represent(s) angular info?

Which represent(s) radial info?

Which orbital is being considered?