Chem 534: Problem Set #5

Due in class: Tues, October 27th

Useful websites for
atoms: http://physics.nist.gov/PhysRefData/Handbook/element_name.htm
diatomic & polyatomic molecules: http://webbook.nist.gov/chemistry & http://cccbdb.nist.gov

(1) Consider the X^2B_1 ground electronic state of the $ClO_2(g)$ molecule. It has a symmetric, bent geometry with bond lengths of 1.470 Å and a bond angle of 117.4º, hence it is an asymmetric top (like water).

(a) Calculate the moment of inertia tensor and diagonalize it to obtain the 3 rotational temperatures of ClO_2. Note that a judicious choice of coordinate system will simplify the form of the tensor.
(If needed, a convenient matrix diagonalization routine can be found on the web at: http://www.bluebit.gr/matrix-calculator/default.aspx)

(b) Calculate the entropy of ClO_2 at 298 K and compare your result to the experimental value of 255 J mol^{-1} K^{-1}. Vibrational frequencies can be found from the NIST Webbook above.

(2) Now consider the closed-shell singlet ground state of $NH_3(g)$.

(a) Calculate the molar constant volume heat capacity of ammonia at 298 K, giving each contribution (translation, vibration, etc.) together with the total.

(b) Calculate the equilibrium constant K_p at 400ºC for $\frac{3}{2}H_2 + \frac{1}{2}N_2 \rightarrow NH_3$.