Chemistry 562 **Spring 2012**

Problem Set 5

Due beginning of class on <u>Friday</u>, February 24th

(Make your reasoning clear. We need to understand your reasoning, not just see the final result.)

1. (a) For a particle with an angular momentum quantum number l=3, work out the magnitude of the angular moment (L) and of its possible projections ($L_z \equiv l_z$) onto the z-axis in units of $\hbar$. Give the angle from the z-axis for the possible values of the projections and sketch a diagram.

   (b) Could we know the projection of L onto the y-axis ($L_y \equiv l_y$) simultaneously with L and L_z? Explain by calculating the commutator.

   (c) Can we know both of the projections onto the l_y and l_x axes? Explain by calculating the commutator.

   (d) Confirm that the wave function for m_l=0 satisfies the Schrödinger equation and find its energy.

2. What is the degeneracy of J=0 and J=1 for a linear, symmetric, and spherical rotor? For each rotor, give the complete set of quantum numbers for each state. (Each state should have a unique set of quantum numbers.)

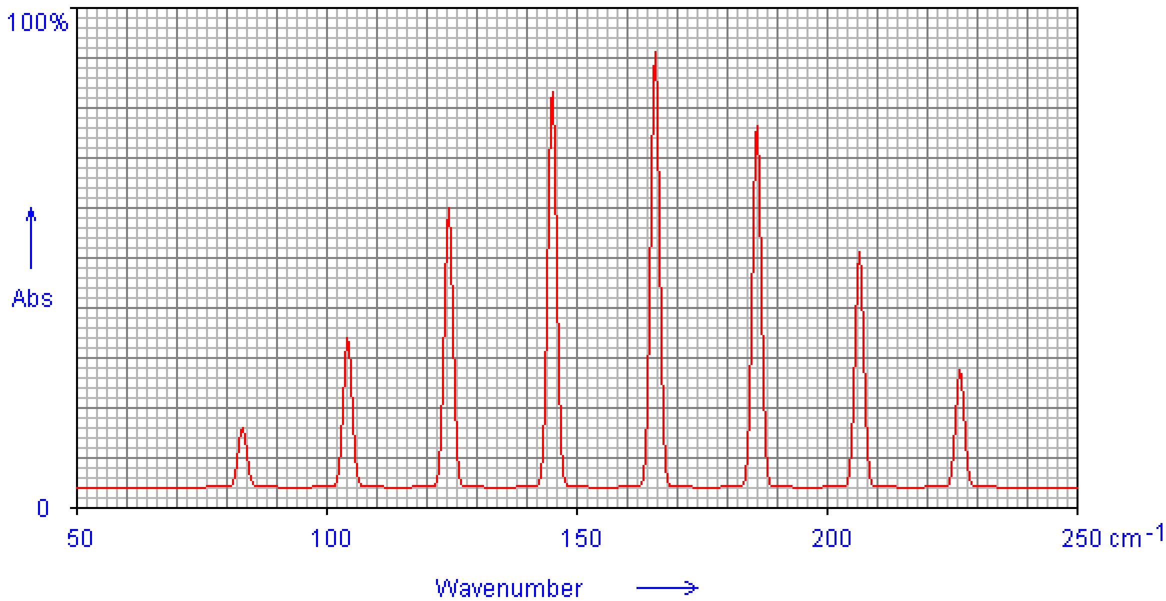
3. (a) What are the selection rules for a pure rotational transition?

   (b) Write the x, y and z components of the transition dipole operator for pure rotations in spherical harmonics.

   (c) Mathematically show that the light-induced transition between the J=0 and J=2, m_J=0 rotational wavefunctions is not allowed. (See Further Information 12.2 for help.)

Problem 4 is on the next page.

4. The rotational spectrum of $H^{35}Cl$ is shown below.



(a) Label each peak with the correct transition $J_u \leftarrow J_L$ transition. Note that the first observable transition is $J_u=4 \leftarrow J_L=3$, because the first two transitions are too weak to observe experimentally.

(b) Determine a rough value for the rotational constant *B* for $H^{35}Cl$ from this spectrum. Give your answer in units of cm^{-1}.

(c) Calculate the equilibrium bond length for $H^{35}Cl$ in Å from your estimate of *B*.