Chem 332: Problem Set #6

Due in class: Wednesday, March 6th

(1) Show that $\left[\ell_x, \ell_z\right] = -i\hbar\ell_y$

(2) The *real* angular functions

$$Y_{xz} = \frac{i}{\sqrt{2}}(Y_{2,1} + Y_{2,-1}) \qquad Y_{yz} = \frac{i}{\sqrt{2}}(Y_{2,1} - Y_{2,-1})$$

$$Y_{xy} = \frac{1}{\sqrt{2}}(Y_{2,2} - Y_{2,-2}) \qquad Y_{z^2} = Y_{2,0} \qquad Y_{x^2-y^2} = \frac{i}{\sqrt{2}}(Y_{2,2} + Y_{2,-2})$$

are often used in discussions of chemical bonding where the Y_{l,m_l} are the usual spherical harmonic functions. The above are the angular factors of atomic *d*-orbital wavefunctions.

(a) Determine if ℓ_z or ℓ^2 are precisely known for a state described by Y_{xy}. If precisely known, make sure to give its value.

(b) Given that $Y_{2,\pm 1} = \mp\frac{1}{2}\left(\frac{15}{2\pi}\right)^{1/2} \sin\theta\cos\theta\, e^{\pm i\phi}$, show that Y_{xz} is pure real.

(c) Confirm that the spherical harmonic $Y_{2,-1}$ satisfies the Schrödinger equation for a particle free to rotate in 3 dimensions. What is its energy?

(3) In the microwave spectrum of $^{12}C^{16}O$, the $J = 0 \rightarrow 1$ transition was measured at 115,217.204 MHz.

(a) Calculate the moment of inertia (in amu Å^2), rotational constant B (in MHz), and the bond length of CO (in Å).

(b) Predict the rotational constant for $^{13}C^{16}O$ (in MHz).

(c) Determine which transition has the maximum intensity in the pure rotational spectrum of $^{12}C^{16}O$ at 300 K.