CHEM 361B - Lecture 11 Activity

The Rigid Rotator and Angular Momentum

1. Table 1 shows the observed microwave adsorption spectrum of $H^{127}I$ and $D^{127}I$ between 60 cm^{-1} and 90 cm^{-1}. Take the mass of ^{127}I to be 126.904 m_u and the mass of D to be 2.013 m_u.

Table 1: Spectral lines for $H^{127}I$ and $D^{127}I$.

	$\frac{1}{\lambda}$ (cm^{-1})			
$H^{127}I$	64.275	77.130	89.985	
$D^{127}I$	65.070	71.577	78.084	84.591

   (a) Is the spacing between each spectral line equal? Is this what you expect?
   (b) Based on the spectra, show that the moment of inertia, I, for $H^{127}I$ is 4.355×10^{-47} kg m^2 and for $D^{127}I$ is 8.60×10^{-47} kg m^2.
   (c) Show that the interatomic distance between $H^{127}I$ is 1.626×10^{-10} m and for $D^{127}I$ is 1.616×10^{-10} m.

2. The results we derived for a rigid rotator apply to linear polyatomic molecules as well as to diatomic molecules.
   (a) Given that the moment of inertia, I, for $H^{12}C^{14}N$ is 1.89×10^{-46} kg m^2, show that the wavenumber of the transition between the rotational ground state and the first excited state is 2.962 cm^{-1}.
   (b) Show that the wavenumber between the $\ell = 1$ to $\ell = 2$ states is 5.924 cm^{-1}
   (c) Using the answer above, sketch the rotational spectrum of $H^{12}C^{14}N$.
   (d) If $H^{12}C^{14}N$ is in the $\ell = 2$ and $m = -1$ state
      i. Show that
      $$Y_2^{-1} = \sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta e^{-i\phi}$$
      Note: $P_\ell^{|m|}(cos\theta)$ means take the appropriate solution to the Legendre functions as a function of $\cos\theta$.
      ii. Show that its energy, $E = 1.767 \times 10^{-22}$ J.
      iii. Show that its total angular momentum, $L = \sqrt{6}\hbar$.
      iv. Show that the z-component to its angular momemtum, $L_z = -\hbar$.

      Hint: Use the eigenfunction/eigenvalue relationship to calculate these values.

3. Show that $P_1^0 = x$ is a solution to the Legendre differential equation
$$(1-x^2)\frac{d^2P}{dx^2} - 2x\frac{dP}{dx} + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right]P(x) = 0$$