1. For nitrogen N\textsubscript{2} and oxygen O\textsubscript{2} molecules

(a) Given that the equilibrium distances of the N-N and O-O are \( r_e = 1.0940 \) Å and 1.2074 Å respectively, calculate their moments of inertia.

(b) Calculate their rotational constants \( B_e \). The measured spectroscopic rotational constants of N\textsubscript{2} and O\textsubscript{2} are \( B_0 = 1.998 \text{ cm}^{-1} \) and \( 1.438 \text{ cm}^{-1} \) respectively. Why is there the difference between \( B_0 \) and \( B_e \)?

(c) Determine the transitions from \( J=0 \) to \( J=1 \) and from \( J=1 \) to \( J=2 \) for both molecules in wave numbers, in megahertz, and in eV.

2. The vibrational energy spacings for the hydrogen halides are

HF: \( 3958.4 \text{ cm}^{-1} \)
HCl: \( 2989.7 \text{ cm}^{-1} \)
HBr: \( 2559.3 \text{ cm}^{-1} \)
HI: \( 2230.0 \text{ cm}^{-1} \)

Calculate the force constant of each hydrogen halide molecule and account for any trend in these force constants.

3. Spectroscopic constants of \(^{127}\text{I}^{35}\text{Cl} \) have been measured: \( \nu_{vib} = 384.18 \text{ cm}^{-1} \) and \( \nu_{vib}x_e = 1.465 \text{ cm}^{-1} \). The bond dissociation energy of \(^{127}\text{I}^{35}\text{Cl} \) has also been measured to be 2.153 eV.

(a) Calculate the wave number of the transition between \( \nu=0 \) and \( \nu=1 \).

(b) Repeat part (a) for the transition between \( \nu=1 \) and \( \nu=2 \).

(c) What is the depth of the molecular potential curve of \(^{127}\text{I}^{35}\text{Cl} \) (that is, what is the value of \( D_e \))?  

4. Consider the HCl molecule and use the following constants for the \( X^1\text{S}^+ \) ground state: \( \nu_{vib} = 2989.74 \text{ cm}^{-1} \), \( \nu_{vib}x_e = 52.05 \text{ cm}^{-1} \), \( \nu_{vib}y_e = 0.056 \text{ cm}^{-1} \), \( B_e = 10.5909 \text{ cm}^{-1} \), \( a_e = 0.3019 \text{ cm}^{-1} \), \( r_e = 1.27460 \) Å (the first electronic excited state lies about 77000 \text{ cm}^{-1} \) above the ground state).

(a) Calculate the rotational constant \( D_e \).

(b) Calculate the first six rotational energy levels (consider the molecule as vibrating rotator).

(c) Calculate the first six vibrational energy levels.

(d) Sketch the vibration-rotation energy levels you have got.
5. Given the following constants for N₂,

<table>
<thead>
<tr>
<th></th>
<th>(\tilde{\nu}_e)</th>
<th>(B_0)</th>
<th>(B_1)</th>
<th>(D_0) (cm(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>N₂</td>
<td>2330.7</td>
<td>1.98957</td>
<td>1.97219</td>
<td>5.76E-6</td>
</tr>
</tbody>
</table>

Where \(\tilde{\nu}_e\) is the vibrational frequency, \(B_0\), \(B_1\) and \(D_0\) are the rotational constants. (All four quantities are in wavenumber (cm\(^{-1}\)) unit.) Shine a 532nm laser beam through a Raman cell containing N₂, and observe the scattering light to an angle perpendicular to the laser beam. Rayleigh, pure rotational Raman, and vibration-rotational Raman scattering lines will occur.

1. What is the Rayleigh scattering light wavelength (nm) and corresponding wavenumber (cm\(^{-1}\))? 

2. Take this Rayleigh scattering light as the reference of wavenumber, figure out the relative wavenumber of pure rotation Raman (RR) lines (originated from \(v = 0\)). Mark the corresponding branch and consider the first 6 lines for each branch.

3. Take this Rayleigh scattering light as the reference of wavenumber, figure out the relative wavenumber of vibration-rotational Raman (VRR) lines (only consider \(v = 0\) and \(v = 1\) vibrational levels and associated rotational levels). Mark the corresponding branch and consider the first 6 lines for each branch.

4. For the vibration-rotational Raman lines, calculate the wavelength of the Q-Branch (0-0) transition lines. [(0-0) means from \(J = 0\) to \(J = 0\)]

5. Assume the transition matrix elements (transition probability) are equal for the Stokes VRR and anti-Stokes VRR, estimate the intensity ratio between the Stokes and the anti-Stokes VRR lines from the Boltzmann factor.