b. What is the value of the anharmonicity constant, $\chi''$?

$$\chi'' = \frac{388.3 \text{ cm}^{-1}}{1.4683 \text{ cm}^{-1}} = 267.0 \text{ cm}^{-1}$$

a. What is the fundamental frequency, $\nu_0$?

$$\nu_0 = \frac{\hbar \omega}{2\pi m}$$

<table>
<thead>
<tr>
<th>$\nu$ (cm$^{-1}$)</th>
<th>575</th>
<th>375.5</th>
<th>376</th>
<th>376.5</th>
<th>377</th>
<th>377.5</th>
<th>378</th>
<th>378.5</th>
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<th>380.5</th>
</tr>
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<td>380</td>
<td>380.5</td>
</tr>
</tbody>
</table>

You are allowed to use a calculator for the exam.

Instructions: You have fifty minutes to complete this exam. Please place your name on all pages of this exam. Exams submitted without a name will not be graded.
For an NMR transition to occur the applied magnetic field (B₀) must be parallel to the electron's magnetic field (B₂). It is not possible to perform NMR spectroscopy on a nucleus with a nuclear spin of zero. 

The dissociation energy of a molecule is measured between the bottom of the potential well of a given electronic state and zero energy where zero energy is defined as the zero point energy of two widely separated atoms.

The zero point energy refers to the energy at the minimum of the potential well of the ground electronic state.

The relative energies of electronic, rotational, and vibrational and NMR transitions are given by the Gouterman-Moore rule or Faust's rule. No credit will be given when the entire word Rule or False of each is given. Determine whether each of the following statements is true or false.

1. Non-zero rotational constants

\[
\frac{2\pi}{\hbar} = \alpha \left[ 1 + \frac{1}{2} \left( \frac{1}{2} + 1 \right) \right]
\]

The perturbing operator for the NMR transition is \( I_x \) or \( I_y \). Show that transitions from \( I_x \) to \( I_y \) lead to \( I_z \) transitions of the form

\[
(2) \frac{\hbar}{\Delta} = \epsilon \hbar
\]

\[
[(2) \sigma^+(1) \sigma^-] = \epsilon \hbar
\]

\[
[(2) \sigma^+(1) \sigma^+] = \epsilon \hbar
\]

\[
(2) \sigma^-(1) \sigma^- = I_z \hbar
\]

Indistinguishable protons. The wave functions of the states are

2. (15 points) Consider performing NMR spectroscopy on a simple system of two coupled...
4. (20 points) A subset of vibrational and rotational energy levels for a generic diatomic molecule are shown below. On the diagram clearly draw and label the following quantities:

e. The zero point energy.
d. The fundamental vibrational frequency. (Assume \( \nu = 0 \) for this portion of the problem.)
c. The first vibrational overtone (Assume \( \nu = 0 \) for this portion of the problem.)
b. The R branch transition which originates from the \( v=0 \), \( J=1 \) level.
a. The P branch transition originating from the \( v=0 \), \( J=1 \) level.

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molecular weight of 17 g/mol (remember N₂I = 6.022 x 10²³ atoms/mol). Clearly, state any assumptions made.

6. (15 points) The microwave spectrum (pure rotational spectrum) of H₂I shows a series of lines.

b. What is the physical significance of the second term, (\varepsilon_2 - \varepsilon_1)?

2. (10 points) In a simple two-level system, the probability of a transition between the two states,

\[ p_{12} = \frac{p_{21}}{1 - p_{21}} \]
\[ \text{Some possibly useful constants: } \hbar = 9.46 \times 10^{-34}, \ \text{MHz} = 5.05 \times 10^{14}, h = 6.626 \times 10^{-34} \text{Js} \]

a. What is the frequency of an \( ^{1}H \) MR transition if the applied magnetic field is 6 T?

\[ \frac{\gamma}{c_0} g_n ^{m_n} \nu_0 = \nu \]

b. Construct an energy level diagram for \( ^{3}H \) in an externally applied magnetic field of 6 T.

\[ \frac{\gamma}{c_0} g_n ^{m_n} \nu_0 = \nu \]

\[ \frac{\gamma}{c_0} g_n ^ {m_n} \nu_0 = \nu \]

\[ z I_0 g_n ^ {m_n} \nu_0 = \nu \]

The nuclear spin states of \( ^{3}H \) can be described in the form of \( I = \frac{1}{2}, m_I \). Even though there are more than two nuclear spin states for \( ^{3}H \) each individual state is still an eigenstate of the nuclear spin angular momentum operator \( I \). Where

\[ \langle I_m I_m | = \delta_{m,m'} \]

\[ \text{The isotope } ^{3}H \text{ can be used in NMR spectroscopy.} \]
The difference between transitions within a given multiplet is roughly 0.03 ppm.

The shielding constant for the two protons is higher than that for the 6 protons.

270 Hz.

The difference in the transition frequency between the two chemical environments is

0.04 ppm.

The multiplet of the 6 protons at the end of the molecule is centered at a chemical shift, assuming the spectrum is experienced by the two different chemical environments. The environment is experienced by the six protons at the ends of the molecule (three on each end) and another chemical environment is

21 Hz.

The spectrum of propene (CH₂CH₂CH₃) is acquired with the molecule in the middle of the molecule.

9. 5 points. Extra credit. Describe the Frank-Condon principle. Use diagrams if necessary.