1a. The eigenvalues of $\hat{H}$ are $2I\hbar^2 l(l+1)$. You can see this from the following argument - suppose $\psi$ is an eigenfunction of $\hat{H}$ with eigenvalue $\lambda$.

$$\hat{H}\psi = \lambda \psi$$

$$2I\hat{\hat{l}}^2 \psi = \lambda \psi$$

$$2I\hbar^2 l(l+1) \psi = \lambda \psi$$

Unfortunately I made an error in constructing this problem. The correct relationship between $\hat{H}$ and $\hat{l}^2$ is $2I\hat{H} = \hat{l}^2$. This error will affect the answers to parts 2d-f.

1b. The operators must share the same eigenfunctions ($\psi$ is part 1a is defined as an eigenfunction of $\hat{H}$, and is shown to be an eigenfunction of $\hat{l}^2$). Operators that share the same eigenfunctions commute (a proof was given in lecture).

1c. The operators can share the same eigenfunctions. A proof of this was given in class. No, we don't expect the operators to share the same eigenvalues. An example of operators that commute, share the same eigenfunctions, but don't share the same eigenvalues is given in part 1a.

2a. $l = 1$ for $p_z (= Y_1^0)$. Also, $l = 1$ for $p_y (= N_y(Y_1^1 - Y_1^{-1}))$. According to the information given in part 1a, the eigenvalues of $\hat{l}^2 = \hbar^2 l(l+1) = 2\hbar^2$ for these functions.

2b. $m_l = 0$ for $p_z (= Y_1^0)$. Based on the information at the top of p. 2, the eigenvalue associated with $p_z$ is $0 \hbar^2$.

$p_y$ is a linear combination of functions with different $m_l$ so it is not an eigenfunction of $\hat{l}_z$. The expectation value $<\hat{l}_z>$ is a weighted average of the different $m_l$ that go into $p_y$. The two functions have $m_l = +1$ and -1, respectively, and these functions contribute equally to the wave function, so $<\hat{l}_z>$ is a simple average of these quantum numbers and $<\hat{l}_z> = 0$.

2c. Many of you pointed out that these operators can share eigenfunctions, but do not need to. That's a good place to start, but I was looking for something that pertained to these particular functions.

The only time when eigenfunctions of one operator do not need to be eigenfunctions of the other is when an eigenfunction of the first operator is a member of a degenerate set. $p_y$ combines spherical harmonics that have the same $l$ and are degenerate eigenfunctions of $\hat{l}$. Because the spherical harmonics have different $m_l$, they are not degenerate eigenfunctions of $\hat{l}_z$, so $p_y$ is not an eigenfunction of the latter operator.

Keep in mind, however, it is always possible to choose a single set of functions that will be eigenfunctions of two commuting operators.

2d. The instructions say to use the eigenvalue formula in part 1a, but as remarked above, this formula was in error. Two solutions are given below:

Starting with formula in part 1a

$$E = 2I\hbar^2 l(l+1)$$
\textbf{In[1]} := \begin{align*}
\text{amu} &= 1.66 \times 10^{-27} \\
mN &= 14.003 \text{ amu} \\
\mu &= \frac{mN^2}{2 mN} \\
r &= 109.8 \times 10^{-12} \\
\text{IN2} &= \mu r^2 \\
hbar &= 1.055 \times 10^{-34}
\end{align*}
\textbf{Out[1]} = 1.66 \times 10^{-27}
\textbf{Out[2]} = 2.3245 \times 10^{-26}
\textbf{Out[3]} = 1.16225 \times 10^{-26}
\textbf{Out[4]} = 1.098 \times 10^{-10}
\textbf{Out[5]} = 1.40121 \times 10^{-46}
\textbf{Out[6]} = 1.055 \times 10^{-34}

\textbf{In[7]} := \begin{align*}
l &= \{0, 1, 2\} \\
\text{Energy} &= 2 \text{ IN2} hbar^2 l (1 + 1)
\end{align*}
\textbf{Out[7]} = \{0, 1, 2\}
\textbf{Out[8]} = \{0, 6.23834 \times 10^{-114}, 1.8715 \times 10^{-113}\}

\textbf{Using the correct formula}

\textbf{In[9]} := \text{Clear[Energy]}
\textbf{Energy} = \frac{hbar^2 l (1 + 1)}{2 \text{ IN2}}
\textbf{Out[10]} = \{0, 7.9433 \times 10^{-23}, 2.38299 \times 10^{-22}\}

\textbf{2e.} The allowed absorption transitions are \(J=0 \to J=1\) and \(J=1 \to J=2\). The transition energies are, depending on your results for \textbf{part 2d},

\textbf{In[11]} := \{6.2383 \times 10^{-114} - 0, 1.8715 \times 10^{-113} - 6.2383 \times 10^{-114}\}
\textbf{Out[11]} = \{6.2383 \times 10^{-114}, 1.24767 \times 10^{-113}\}

\textbf{or}

\textbf{In[12]} := \{7.9433 \times 10^{-23} - 0, 2.3830 \times 10^{-22} - 7.9433 \times 10^{-23}\}
\textbf{Out[12]} = \{7.9433 \times 10^{-23}, 1.58867 \times 10^{-22}\}

\textbf{2f.} Depending on your results for \textbf{part 2d}, two different rotational constants are possible.

First, accepting the error in \textbf{part 1a}, you obtain \(hcB = 2l hbar^2\), or \(B = \frac{l hbar}{\pi c}\)
Second, using the correct formula, $\hbar cB = \hbar^2 \frac{\ell^2}{2I}$, or $B = \frac{\hbar c}{4\pi c I}$.

3a. The boundary condition for the harmonic oscillator wave functions is that the wave functions vanish as $x$ goes to one extreme value ($+\infty$) or the other ($-\infty$).

3b. The boundary condition for the 2D rigid rotor wave functions is that they be periodic in $\phi$ with a period of $2\pi$. That is, $\psi(\phi) = \psi(\phi + 2\pi)$.

4a. To evaluate the transition dipole moment using the operator provided requires two integrals:

$$
\mu_{02}^0 = \mu_{x=0} \int y_0 \psi_2 \, d\ell x + (\frac{d\mu}{d\ell x})_{x=0} \int y_0 x \psi_2 \, d\ell x
$$

4b. The first integral in part 4a is just an overlap integral. This integral vanishes because the wave functions are eigenfunctions of the same operator and are orthogonal.

The second integral contains 3 items with different symmetry: $y_0$ (even symmetry), $x$ (odd symmetry), and $\psi_2$ (even symmetry). Taken together, the collected function has odd symmetry, so its integral vanishes.

4c. The $v=0 \rightarrow v=1$ transition is accompanied by a change in rotational state, with loss of rotational energy, and gain of rotational energy, both being possible. The allowed transitions are $\Delta \ell = +1$ and -1, and each allowed transition occurs at a different energy. Many rotational states are populated at room temperature, so many peaks appear in the spectrum.

The peak intensities reflect the populations of the starting rotational energy states, that is, the states with the largest populations produce the most intense peaks. The lowest energy rotational states, which produce the peaks near the center of the pattern, do not have the highest populations because they have low degeneracy. States of slightly higher energy have higher populations because they are much higher degeneracy.

4d. According to the harmonic oscillator model, the first overtone should occur at exactly twice the fundamental frequency, $4300 \text{ cm}^{-1}$. According to the anharmonic model, $\Delta E_{10} > \Delta E_{21}$, so the first overtone transition ($v=0$ to $v=2$) should require less energy than two $v=0$ to $v=1$ transitions, and the first overtone frequency should be smaller than $4300 \text{ cm}^{-1}$.