Homework #1 Key

(1.) $\tilde{\nu} = 2349.16\ cm^{-1}$

ν

$\nu = c/\lambda$

$c = 2.9979 \times 10^{10}\ cm/s$

$\lambda = 0.0004257\ cm$

$\boxed{\nu = 7.04255 \times 10^{13}\ Hz}$

λ

$\lambda = 1/\tilde{\nu} = 0.0004257\ cm$

$1\ cm = 10^7\ nm$

$\boxed{\lambda = 4256.84\ nm}$

E

$E = h\nu$

$\nu = 7.04255 \times 10^{13}\ Hz$

$h = 6.626076 \times 10^{-34}\ J \cdot s$

$\boxed{E = 4.66645 \times 10^{-20}\ J}$

(2.) $k_{^{79}Br\,^{79}Br} = 240\ N \cdot m^{-1}$

a.) $\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{79.79}{79+79} = 39.5\ amu \times \frac{1.66 \times 10^{-27}\ kg}{1\ amu} = \boxed{6.557 \times 10^{-26}\ kg}$

$\nu = \frac{1}{2\pi}\left(\frac{k}{\mu}\right)^{1/2} = \frac{1}{2\pi}\left(\frac{240}{6.557 \times 10^{-26}}\right)^{1/2} = 9.63 \times 10^{12}\ Hz$ or $321.2\ cm^{-1}$

$\mathcal{E}_0 = \frac{1}{2} h\nu = \frac{1}{2}(6.626 \times 10^{-34}\ J \cdot s)(9.63 \times 10^{12}\ s^{-1}) = \boxed{3.19 \times 10^{-21}\ J}$

b.) Because N≡N is a triple bond and Br_2 is a single bond. The triple bond is a tighter spring and therefore has a higher spring constant.

(3) $\tilde{\nu} = 2330\ cm^{-1}$, $D_0 = 78715\ cm^{-1}$ for N_2

$D_e = D_0 + \frac{h\nu}{2}$

$\tilde{\nu} = \nu/c$ or $\nu = c\tilde{\nu} = 2.9979 \times 10^{10}\ cm/s \times 2330\ cm^{-1} = 6.985 \times 10^{13}\ Hz$

$\frac{h\nu}{2} = \frac{(6.626 \times 10^{-34}\ J \cdot s)(6.985 \times 10^{13}\ s^{-1})}{2} = 2314 \times 10^{-20}\ J$ or $1165\ cm^{-1}$

$D_0 \Rightarrow E = hc\tilde{\nu} = 1.5436 \times 10^{-18}\ J$

$D_e = D_0 + h\nu/2 = \boxed{1.5867 \times 10^{-18}\ J \text{ or } 79880\ cm^{-1}}$

4.

$$E = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$$

(m ↑ mass of e^-)

- ground state is $n_x = n_y = n_z = 1$
- cube, therefore $a = b = c = 1\,nm$ $(1 \times 10^{-9}\,m)$

$$E = \frac{(6.626 \times 10^{-34}\ J \cdot s)^2}{8 \cdot (9.109 \times 10^{-31}\ kg)}\left(3 \cdot \frac{1}{(10^{-9}\ m)^2}\right)$$

recall, $J = \frac{kg\ m^2}{s^2}$

$$\boxed{E = 1.81 \times 10^{-19}\ J}$$

5.

Part	molecule	Total DoF	TRANS	ROT	VIB
a	CH_3Cl	15	3	3	15-6=9
Linear b	OCS	9	3	2	9-5=4
c	C_6H_6	36	3	3	36-6=30
d	H_2CO	12	3	3	12-6=6

6.

a) $\varepsilon_0 = 0$ $\quad \varepsilon_1 = \frac{\hbar^2}{I}$ $\quad \varepsilon_2 = \frac{3\hbar^2}{I}$

$\Delta\varepsilon_{0\to1} = \frac{\hbar^2}{I}$ $\quad \Delta\varepsilon_{0\to2} = \frac{3\hbar^2}{I}$ $\quad \therefore\ \Delta\varepsilon_{0\to2} = 3\,\Delta\varepsilon_{0\to1}$

$\Delta\nu_{0\to2} = 3(1.153 \times 10^{11}\ Hz) = \boxed{3.459 \times 10^{11}\ Hz}$

$\Delta E_{0\to2} = 2.29 \times 10^{-22}\ J = \boxed{2.29 \times 10^{-25}\ kJ}$

$\Delta\lambda_{0\to2} = \boxed{8.66695 \times 10^{5}\ nm}$

$\Delta\tilde{\nu}_{0\to2} = \boxed{11.54\ cm^{-1}}$

b) $g_J = 2J + 1$

Level	g_J
J = 0	1
J = 1	3
J = 2	5
J = 3	7