VP390 Problem Set 8

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1 Problem 1

$$U^{\dagger}U = UU^{\dagger} = I_n$$
$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\mathbf{Pr}(|\psi_1\rangle = |1\rangle) = a^2$$
$$\mathbf{Pr}(|\psi_1\rangle = |0\rangle) = b^2$$

$$\frac{\mathrm{d}U(r)}{\mathrm{d}r} = U_0[-12\frac{a^{12}}{r^{13}} + 6(\frac{a^6}{r^7})] = 0$$
$$r^6 = 2a^6 \rightarrow r_0 = \sqrt[6]{2}a$$
$$U(r_0) = -\frac{U_0}{4}$$

2 Problem 2

(a)

$$E_{el} = -\frac{1}{4\pi\varepsilon_0}\frac{q_1q_2}{r} + E_{Na+} - E_{Cl-} = -\frac{1.44}{0.24} + 5.14 - 3.62 = -4.48\text{eV}$$

(b)

$$E_{ex} = |E_{el}| - |E_d| = 4.48 - 4.27 = 0.21\text{eV}$$

(c)

$$E_{ex} = \frac{A}{r^n} = \frac{1}{4\pi\varepsilon_0}\frac{q_1q_2}{r} + E_{Na+} - E_{Cl-}$$

Since it's in equilibrium position, the two forces are equal

$$\frac{1}{4\pi\varepsilon_0}\frac{q_1q_2}{r_0^2} = \frac{n}{r_0}\frac{A}{r_0^n}$$

$$\frac{1.44}{0.24^2} = 0.21\frac{n}{0.24} \rightarrow n \approx 29, A \approx 2.23 \times 10^{-19}\text{eVnm}^2$$

3 Problem 3

$$\rho_{ionic} = er_0 = 1.6 \times 10^{-19} \times 0.0917 \times 10^{-9} = 1.4672 \times 10^{-29}\text{Cm}$$

$$\frac{\rho_{measure}}{\rho_{ionic}} = \frac{6.4 \times 10^{-30}}{1.4672 \times 10^{-29}} \approx 43.6\%$$

4 Problem 4

$$\rho_{ionic} = er_0 = 1.6 \times 10^{-19} \times 0.193 \times 10^{-9} = 3.088 \times 10^{-29}\text{Cm}$$

$$\frac{\rho_{measure}}{\rho_{ionic}} = \frac{26.7 \times 10^{-30}}{3.088 \times 10^{-29}} \approx 86.5\%$$

5 Problem 5

(a)

$$E = h\nu = h\frac{c}{\lambda} \to \lambda = h\frac{c}{E} = 6.63 \times 10^{-34}\frac{3 \times 10^8}{0.3 \times 1.6 \times 10^{-19}} \approx 4.14 \times 10^{-6}\text{m}$$

(b) Since $\lambda > 1000nm$, it belongs to Paschen part of the spectrum, and it's infrared ray

(c) Because the bond strength only accounts for 15% of the total bond, and others are are not broken

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(a)

$$\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{35.5 \times 39}{35.3 + 39} \times 1.66 \times 10^{-27} \approx 3.08 \times 10^{-26}\text{kg}$$

(b)

$$I = \frac{\hbar^2}{2E_{rot}} = \frac{(1.05 \times 10^{-34})^2}{2 \times 1.43 \times 10^{-5} \times 1.6 \times 10^{-19}} \approx 2.41 \times 10^{-45}$$

$$r_0 = \sqrt{\frac{I}{\mu}} \approx 2.8 \times 10^{-10}\text{m}$$

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$$k = (2\pi f)^2 \frac{m_N m_O}{m_N + m_O} = (2 \times \pi \times 5.63 \times 10^{13})^2 \frac{14 \times 16}{14 + 16} \times 1.66 \times 10^{-27} \approx 1551\text{N/m}$$

8 8

(a)

$$\mu = \frac{m_C m_O}{m_C + m_O} = \frac{12 \times 16}{12 + 16} \times 1.66 \times 10^{-27} \approx 1.34 \times 10^{-26}$$
$$I = \mu r_0^2 = 1.34 \times 10^{-26} \times (0.113 \times 10^{-9})^2 \approx 1.45 \times 10^{-46} kg \cdot m^2$$
$$E_{0r} = \frac{\hbar^2}{2I} = \frac{(1.05 \times 10^{-34})^2}{2 \times 1.45 \times 10^{-46}} \approx 2.37 \times 10^{-4}\text{eV}$$

(b)

$$\omega = \sqrt{\frac{2E_{0r}}{I}} = \sqrt{\frac{2 \times 2.37 \times 10^{-4} \times 1.6 \times 10^{-19}}{1.45 \times 10^{-46}}} \approx 7.23 \times 10^{11}\text{rad/s}$$

For $\nu = 0$:

$$E_{\nu=0} = \hbar\omega(0 + 1/2) = 1.05 \times 10^{-34} \times 7.23 \times 10^{11} \times 0.5 \approx 3.8 \times 10^{-23}\text{J} = 2.37 \times 10^{-4}\text{eV}$$

Hence for $l = 1, \nu = 0, E = 2.37 \times 10^{-4} + 2 \times 2.37 \times 10^{-4} = 7.11 \times 10^{-4}\text{eV}$
For $l = 2, \nu = 0, E = 1.659 \times 10^{-3}\text{eV}$
For $l = 3, \nu = 0, E = 3.081 \times 10^{-3}\text{eV}$
For $l = 4, \nu = 0, E = 4.977 \times 10^{-3}\text{eV}$
For $l = 5, \nu = 0, E = 7.347 \times 10^{-3}\text{eV}$

(c) $\triangle E_{5\to4} = 2.37 \times 10^{-3}\text{eV}$
$\triangle E_{4\to3} = 1.896 \times 10^{-3}\text{eV}$
$\triangle E_{3\to2} = 1.422 \times 10^{-3}\text{eV}$
$\triangle E_{2\to1} = 9.48 \times 10^{-4}\text{eV}$
$\triangle E_{1\to0} = 4.74 \times 10^{-4}\text{eV}$

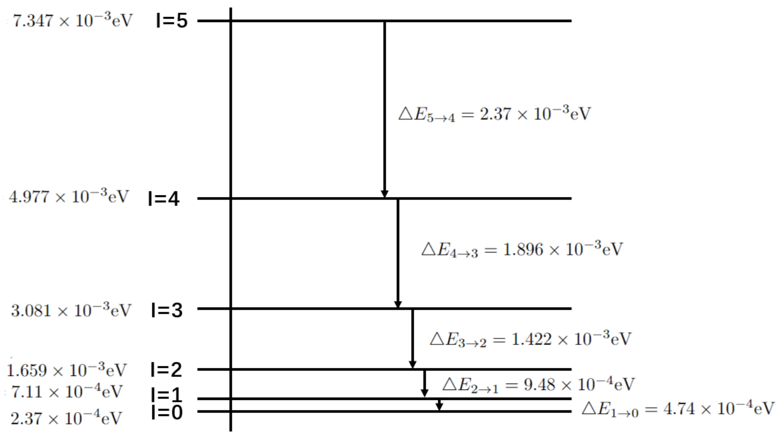

Figure 1: Energy Diagram when $\nu = 0$

(d)

$$\lambda_{l+1} = h\frac{c}{E_{l+1\to l}} = \frac{1.989 \times 10^{-25}}{1.6 \times 10^{-19} \times (l+1)(1.05 \times 10^{-34})^2/(1.45 \times 10^{-46})}$$
$$\triangle\lambda_1 = 2.62 \times 10^{-3}\text{m}$$

$$\triangle\lambda_2 = 1.31 \times 10^{-3}\text{m}$$
$$\triangle\lambda_3 = 8.74 \times 10^{-3}\text{m}$$
$$\triangle\lambda_4 = 6.56 \times 10^{-4}\text{m}$$
$$\triangle\lambda_5 = 5.25 \times 10^{-4}\text{m}$$

All light are in microwave.