phy130B F08

HW9 Solution

Molecules

#1. For rotational energy $E \propto \frac{\hbar^2}{\mu R^2}$, in our case, for HCl, $\mu \sim M_H$.

$\Rightarrow E_r = E_e \frac{m_e}{m_H} \Rightarrow$ using $E = \frac{hc}{\lambda} \Rightarrow \lambda^{-1} = 100\,cm^{-1} \Rightarrow$ it's rotational transition

$\Delta k$ for this problem is $103.73 - 83.03 = 20.7$, $124.3 - 103.73 = 20.57$, $145.05 - 124.3 = 20.75$; $165.51 - 145.05 = 20.46$

$185.86 - 165.51 = 20.35$ so $\Delta k_{avg} = 20.5\,cm^{-1} = \frac{\hbar}{Ic}$ $\Rightarrow I = \frac{\hbar}{\Delta k c} \sim 10^{-46}\,kg\cdot m^2$

The energy transition from $j+1 \rightarrow j$ is $\Delta E = \frac{\hbar^2}{2I}[(j+1)(j+2) - (j+1)j] = \frac{\hbar^2}{I}(j+1) = \hbar kc$

$\Rightarrow k = \frac{\hbar}{Ic}(j+1) \Rightarrow \frac{k}{\hbar/Ic} = j+1 \Rightarrow j = 3.$

$I = \mu R^2 \Rightarrow R = \sqrt{\frac{I}{\mu}} = \sqrt{\frac{I(m_H + m_{cl})}{m_H m_{cl}}} \sim 3\times 10^{-10}\,m$

#2. $E = \frac{l(l+1)\hbar^2}{2I}$ degenercy $= 2j+1$

using Boltzman distribution $N = \frac{(2j+1)e^{-\beta E_j}}{Z}$, $E_j = \frac{\hbar^2}{2I}j(j+1)$, $\beta = \frac{1}{k_B T}$, $k_B T \sim \frac{1}{40}\,eV$

$$\text{Ratio} = \frac{N(j_{10})}{N(j_0)} = \frac{21\, e^{-E_{10}\beta}}{e^{-E_0\beta}} = 21 e^{-\beta(E_{10} - E_0)} \simeq 8.8$$

where $E_{10} = 21.7\,meV$ $E_0 \doteq 0$

T. D. P. T

#1. $C_{2p}(t\to\infty) = \frac{1}{i\hbar}\int_0^\infty dt\, e^{i\omega_{21}t} \langle \phi_{21m} | V_{int} | \phi_{100} \rangle$ where $V_{int} = eE_0 z e^{-\gamma t}$, $z = r\cos\theta$

$$C_{2p}(t\to\infty) = \frac{1}{i\hbar}\int_0^\infty dt\, e^{-t(\gamma - i\omega_{21})} \int_0^\infty r^2 dr\, r R_{21}^* R_{10} \int Y_{1m}^* Y_{00}\cos\theta\, d\Omega = \frac{2^{15/2}}{3^5}\frac{eE_0 a_0}{i\hbar(\gamma - i\omega_{21})}\delta_{m0}$$

$$\Rightarrow P = |C_{2p}(t\to\infty)|^2 = \frac{2^{15}}{3^{10}}\frac{e^2 E_0^2 a_0^2}{\hbar^2(\gamma^2 + \omega_{21}^2)}\delta_{m0}$$

#2. $C_1(\tau) = \frac{1}{i\hbar}\int_0^\tau dt\, e^{i\omega_{10}t}\langle 1|W|0\rangle$ $W = -e\xi x = -e\xi\sqrt{\frac{\hbar}{2m\omega}}(A + A^+)$

$$= \frac{ie\xi}{\sqrt{2m\hbar\omega}}\int_0^\tau dt\, e^{i\omega_{10}t}\langle 1|A + A^+|0\rangle$$

$$= \frac{e\xi}{\sqrt{2m\hbar\omega}}\frac{1}{\omega_{10}}(e^{i\omega_{10}\tau} - 1)$$

for 1D.H.O. $\omega_{n,n-1} = \frac{E_n - E_{n-1}}{\hbar} = \omega$

$$= \frac{e\xi}{\sqrt{2m\hbar}\,\omega^{3/2}}(e^{i\omega\tau} - 1)$$

$$\Rightarrow P = |C_1(\tau)|^2 = \frac{2e^2\xi^2}{m\hbar\omega^3}\sin^2\left(\frac{\omega\tau}{2}\right)$$

$C_2^{(1)}(\tau) \propto \langle 2|x|0\rangle = 0$

$$C_2^{(2)}(\tau) = \frac{1}{\hbar^2}\sum_{j\neq 0}\int_0^\tau dt'\, e^{i\omega_{2j}t'}\langle 2|W|j\rangle\int_0^{t'} dt\, e^{i\omega_{j0}t}\langle j|W|0\rangle$$

$$= \frac{-e^2\xi^2}{2m\hbar\omega}\int_0^\tau dt'\, e^{i\omega t'}\langle 2|A + A^+|1\rangle\int_0^{t'} dt\, e^{i\omega t}\langle 1|A + A^+|0\rangle$$

$$= \frac{e^2\xi^2}{\hbar m\omega^3}\frac{e^{i\omega\tau}}{\sqrt{2}}(\cos(\omega\tau) - 1) \Rightarrow P = |C_2^{(2)}(\tau)|^2 = \frac{e^4\xi^4}{2m^2\hbar^2\omega^6}(\cos(\omega\tau) - 1)^2$$