Quiz #2 Week: Sept. 5 -Sept. 7

Name _____ Chemistry 331

Equations:

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \quad , \quad \nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \quad , \quad E = \frac{h^2 n^2}{8mL^2}$$

1. The vibrational frequency of O_2 is approximately 1580 cm^{-1}. Estimate the vibrational frequency of $^{18}O_2$.

Solution: Use the reduced mass of $^{18}O_2$ and the inverse square root dependence of the frequency to calculate the shifted frequency.

$$\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{m_1 m_1}{m_1 + m_1} = \frac{m_1}{2} = \frac{16}{2} = 8$$

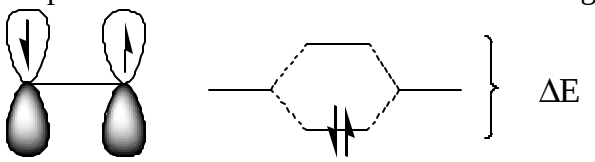
$$\mu' = \frac{m_1}{2} = \frac{18}{2} = 9$$

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \; , \; \nu' = \frac{1}{2\pi}\sqrt{\frac{k}{\mu'}} \; , \; \frac{\nu'}{\nu} = \sqrt{\frac{\mu}{\mu'}}$$

$$\nu' = \nu\sqrt{\frac{\mu}{\mu'}} = 1580\ cm^{-1}\sqrt{\frac{8}{9}} = 1490\ cm^{-1}$$

Frequency in cm^{-1} = _____.

2. Treat the p-electrons of the molecule ethylene as a particle in a box. Assume that the length of box is L = 3 Å. There are two p-electrons as shown in the figure below. Using the particle-in-a-box model calculate the energy difference ΔE.



Solution:

$$E = \frac{h^2 n^2}{8mL^2}$$

$$so\ \Delta E = \frac{h^2}{8mL^2}\left(n_2^2 - n_1^2\right)$$

$$= \frac{\left(6.626\ x\ 10^{-34}\ Js\right)^2}{8\left(9.1\ x\ 10^{-31}\ kg\right)\left(3\ x\ 10^{-10} m\right)^2}\left(4 - 1\right)$$

$$= 2\ x\ 10^{-18}\ J$$

$$\frac{\Delta E}{hc} = 101{,}470\ cm^{-1}$$

$$\lambda = \frac{10^7\ nm\ cm^{-1}}{101{,}470\ cm^{-1}} = 98\ nm$$