Student Number:______________________ Name: ______________________________

# Quiz 3

FYI: $h = 6.626 \cdot 10^{-34}$ J·s; $\hbar = 1.055 \cdot 10^{-34}$ J·s; 1 u = $1.66 \cdot 10^{-27}$ kg; $c = 2.998 \cdot 10^{8}\ \frac{\text{m}}{\text{s}} = 2.998 \cdot 10^{10}\ \frac{\text{cm}}{\text{s}}$

1. **The eigenfunctions of the harmonic oscillator include a special function called**
   (a) Laguerre Polynomial (b) Gauss-Euler function (c) sine/cosine
   (d) Legendre Polynomial (e) Hermite Polynomial (f) Jacobi polynomial

2. **As the reduced mass of a diatomic molecule <u>increases</u>, its vibrational zero-point energy**
   (a) increases (b) decreases (c) does not change.

3. For the particle-in-a-box, the formula for the eigenvalues is $E_n = h^2 n^2 / \left(8ma^2\right)$ **What is the analogous formula for the eigenvalues of the Harmonic Oscillator? Express your answer using** $\hbar, k, \mu$**, where *k* is the force/spring constant for the oscillator and** $\mu$ **is the reduced mass of the oscillator.**

   $E_n =$

4. **The transition from the ground to the first-excited vibrational state in $H_2$, is associated with a spectral line that, in wavenumbers, has the frequency** $\bar{\nu} = 1/\lambda = 4159\ \text{cm}^{-1}$**. What is the vibrational frequency for $D_2$?**

**BONUS:** The equilibrium bond length for the hydrogen molecule is $.7416 \cdot 10^{-10}$ m. What is the frequency, expressed in wavenumbers ($\bar{\nu} = 1/\lambda$; give your answer in units of $\text{cm}^{-1}$) associated with the lowest-energy rotational transition, $J = 0 \rightarrow J = 1$? Assume the rigid rotor approximation is acceptable.

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2. **As the reduced mass of a diatomic molecule <u>increases</u>, its vibrational zero-point energy**
   (a) increases **(b) decreases** (c) does not change.
3. For the particle-in-a-box, the formula for the eigenvalues is $E_n = h^2 n^2 \big/ \left(8ma^2\right)$ **What is the analogous formula for the eigenvalues of the Harmonic Oscillator? Express your answer using $\hbar, k, \mu$, where $k$ is the force/spring constant for the oscillator and $\mu$ is the reduced mass of the oscillator.**

$$E_n = \hbar\sqrt{\tfrac{k}{\mu}}\left(n+\tfrac{1}{2}\right) = \tfrac{1}{2}\hbar\sqrt{\tfrac{k}{\mu}}\left(2n+1\right)$$

4. **The transition from the ground to the first-excited vibrational state in $H_2$, is associated with a spectral line that, in wavenumbers, has the frequency $\bar{\nu} = 1/\lambda = 4159\ \text{cm}^{-1}$. What is the vibrational frequency for $D_2$?**

The transition frequency/wavenumber is given by the difference in energy:

$$E_1 - E_0 = \hbar\sqrt{\frac{k}{\mu}} = h\nu = \frac{hc}{\lambda} = hc\bar{\nu}$$

$$\bar{\nu} = \frac{\hbar}{hc}\sqrt{\frac{k}{\mu}}$$

Using this equation,

$$\frac{\bar{\nu}_{D_2}}{\bar{\nu}_{H_2}} = \frac{\dfrac{1}{2\pi c}\sqrt{\dfrac{k}{\mu_{D_2}}}}{\dfrac{1}{2\pi c}\sqrt{\dfrac{k}{\mu_{H_2}}}} = \sqrt{\frac{\mu_{H_2}}{\mu_{D_2}}} = \sqrt{\frac{\frac{1\text{ u}\cdot 1\text{ u}}{1\text{ u}+1\text{ u}}}{\frac{2\text{ u}\cdot 2\text{ u}}{2\text{ u}+2\text{ u}}}} = \frac{1}{\sqrt{2}}$$

$$\bar{\nu}_{D_2} = \frac{\bar{\nu}_{H_2}}{\sqrt{2}} = \frac{4159\ \text{cm}^{-1}}{\sqrt{2}} = 2941\ \text{cm}^{-1}$$

**BONUS:** The equilibrium bond length for the hydrogen molecule is $.7416 \cdot 10^{-10}$ m. What is the frequency, expressed in wavenumbers ($\bar{\nu} = 1/\lambda$; give your answer in units of $\text{cm}^{-1}$) associated with the lowest-energy rotational transition, $J = 0 \rightarrow J = 1$? Assume the rigid rotor approximation is acceptable.

The rotational levels are given by $E_{\text{rot}}\left(J\right) \equiv \frac{\hbar^2 J\left(J+1\right)}{2\mu r_e^2}$. So the change in rotational energy is

$$\Delta E = E_{\text{rot}}\left(J=1\right) - E_{\text{rot}}\left(J=0\right) = E_{\text{rot}}\left(J=1\right) = \tfrac{\hbar^2 2}{2\mu r_e^2} = \tfrac{\hbar^2}{\mu r_e^2}$$

Using the same equation as from #4,

$$\Delta E = hc\bar{\nu}$$

$$\bar{\nu} = \frac{\hbar^2}{hc\mu r_e^2} = \frac{h^2}{\left(2\pi\right)^2 hc\mu r_e^2} = \frac{h}{\left(2\pi\right)^2 c\mu r_e^2}$$

$$= \frac{6.626 \cdot 10^{-34}\text{kg m}^2\text{s}^{-1}}{\left(2\pi\right)^2\left(\dfrac{1\text{ u}\cdot 1\text{ u}}{1\text{ u}+1\text{ u}}\right)\left(1.66\cdot 10^{-27}\text{kg}\right)\left(2.998\cdot 10^{10}\ \frac{\text{cm}}{\text{s}}\right)\left(.7416\cdot 10^{-10}\text{m}\right)^2} = 122.6\ \text{cm}^{-1}$$