Student Number:______________________ Name: ______________________________

Quiz 6

FYI: $h = 6.626 \cdot 10^{-34}$ $\text{J} \cdot \text{s}$; $\hbar = 1.055 \cdot 10^{-34}$ $\text{J} \cdot \text{s}$; 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 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 cm^{-1}**) associated with the lowest-energy rotational transition,** $J = 0 \rightarrow J = 1$**?** Assume the rigid rotor approximation is acceptable.

2,3. A photon has a wavenumber of $k = \frac{2\pi}{\lambda} = 10^{7}\,\text{m}^{-1}$**.**

(a) What is the momentum of the photon?

(b) What is the energy of the photon?

4. **Show that the eigenvalues of a Hermitian operator are always real.**

Student Number:______________________ Name: ______________________________

Quiz 6

FYI: $h = 6.626\cdot10^{-34}$ J·s; $\hbar = 1.055\cdot10^{-34}$ J·s; 1 u = $1.66\cdot10^{-27}$ kg; $c = 2.998\cdot10^{8}\ \frac{\text{m}}{\text{s}} = 2.998\cdot10^{10}\ \frac{\text{cm}}{\text{s}}$

1. The equilibrium bond length for the hydrogen molecule is $.7416\cdot10^{-10}$ m. What is the frequency, expressed in wavenumbers ($\bar{\nu} = 1/\lambda$; give your answer in units of cm^{-1}) associated with the lowest-energy rotational transition, $J = 0 \to J = 1$? Assume the rigid rotor approximation is acceptable.

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

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

Using the equation for the change in energy in terms of wavenumber,

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

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

$$= \frac{6.626\cdot10^{-34}\text{kg m}^2\text{s}^{-1}}{(2\pi)^2\left(\frac{1\text{ u}\cdot1\text{ u}}{1\text{ u}+1\text{ u}}\right)\left(1.66\cdot10^{-27}\text{kg}\right)\left(2.998\cdot10^{10}\ \frac{\text{cm}}{\text{s}}\right)\left(.7416\cdot10^{-10}\text{m}\right)^2}$$

$$=122.6\text{ cm}^{-1}$$

2. A photon has a wavenumber of 10^7 m^{-1}.

(a) What is the momentum of the photon?

$$p = \hbar k = 1.055\cdot10^{-27}\ \frac{\text{kg}\cdot\text{m}}{\text{s}}$$

(b) What is the energy of the photon?

$$E = h\nu = \frac{hc}{\lambda} = pc = 1.055\cdot10^{-27}\ \frac{\text{kg}\cdot\text{m}}{\text{s}}\cdot 2.998\cdot10^{8}\ \frac{\text{m}}{\text{s}}$$

$$= 3.163\cdot10^{-19}\ \frac{\text{kg}\cdot\text{m}^2}{\text{s}^2}$$

4. **Show that the eigenvalues of a Hermitian operator are always real.**

Let $\hat{C}$ be a Hermitian operator. Then, by definition,

$$\int\left(\hat{C}\Psi_1(x)\right)^*\Psi_2(x)\,dx = \int\Psi_1(x)\hat{C}\Psi_2(x)\,dx$$

Furthermore, let γ_k and $\psi_k(x)$ be eigenfunctions of $\hat{C}$. Then, by definition,

$$\hat{C}\psi_k(x) = \gamma_k\psi_k(x)$$

Taking the complex conjugate of both sides of this equation, we have

$$\left(\hat{C}\psi_k(x)\right)^* = \gamma_k^*\psi_k^*(x)$$

Student Number:______________________ Name: ______________________________

Multiply the first equation on both sides $\psi_k^*(x)\times$ and integrate; multiply the second equation on both sides by $\times\psi_k(x)$ and integrate. (The multiplication sign is used to indicate which side of the expression one multiplies on.) So we have:

$$\int \psi_k^*(x)\hat{C}\psi_k(x)\,dx = \gamma_k \int \psi_k^*(x)\psi_k(x)\,dx$$

$$\int \left(\hat{C}\psi_k(x)\right)^* \psi_k(x)\,dx = \gamma_k^* \int \psi_k^*(x)\psi_k(x)\,dx$$

Rearranging, we can rewrite this as:

$$\frac{\int \psi_k^*(x)\hat{C}\psi_k(x)\,dx}{\int \psi_k^*(x)\psi_k(x)\,dx} = \gamma_k$$

$$\frac{\int \left(\hat{C}\psi_k(x)\right)^* \psi_k(x)\,dx}{\int \psi_k^*(x)\psi_k(x)\,dx} = \gamma_k^*$$

However, because $\hat{C}$ is Hermitian, the left-hand-sides of these equations are the same, and therefore their right-hand sides must also be equal. So $\gamma = \gamma^*$. But any number that is its own complex conjugate must be real (i.e. $(a+bi) = (a+bi)^* = a-bi$ only if $b = \text{Im}[a+bi] = 0$). So the eigenvalues of a Hermitian operator are always real.