

8-14

$$I = \mu r^2 = 1.73 \times 10^{-26} \times (192.6 \times 10^{-12})^2 = 6.4 \times 10^{-46} \text{ kg/m}^2$$

$$B = \frac{h}{8\pi^2 I c} = 0.437 \text{ cm}^{-1} \rightarrow 0.437 \times 3 \times 10^{10} = 1.31 \times 10^{10} \text{ s}^{-1}$$

Line spacing =  $2B = 2.62 \times 10^{10} \text{ s}^{-1}$

8-25

$$\frac{\nu_D}{\nu_H} = \sqrt{\frac{\mu_{\text{CH}_2-\text{CH}_2}}{\mu_{\text{CD}_2-\text{CD}_2}}} = \sqrt{\frac{\frac{(14.01)^2}{28.02} \text{ amu}}{\frac{(16.02)^2}{32.04} \text{ amu}}} = 0.935$$

8-37

$$T = \frac{(2J_{\max} + 1)^2 \hbar^2}{4Ik}$$

First plot

$$J_{\max} = 2 \Rightarrow T = 190 \text{ K}$$

Assuming  $\pm 0.5$  uncertainty in  $J_{\max}$ , and considering the resulting T if  $J_{\max}$  was 1 or 3 (adjacent values to  $J_{\max} = 2$ ), the uncertainty in T is around  $\pm 70 \text{ K}$ .

Second plot

$$J_{\max} = 3 \Rightarrow T = 372 \text{ K}$$

Again assuming  $\pm 0.5$  uncertainty in  $J_{\max}$ , and considering the resulting T if  $J_{\max}$  was 2 or 4 (adjacent values to  $J_{\max} = 3$ ), the uncertainty in T is around  $\pm 120 \text{ K}$ .

9-2

$$\begin{aligned} \frac{d}{dr} \left[ r^2 \frac{dR(r)}{dr} \right] &= \frac{d}{dr} \left[ \frac{r^2}{a_0} e^{-\frac{r}{2a_0}} - \frac{r^3}{2a_0^2} e^{-\frac{r}{2a_0}} \right] \\ &= \frac{1}{a_0} \frac{d}{dr} \left[ r^2 e^{-\frac{r}{2a_0}} - \frac{r^3}{2a_0} e^{-\frac{r}{2a_0}} \right] = \frac{1}{a_0} \left[ 2r e^{-\frac{r}{2a_0}} - \frac{r^2}{2a_0} - \frac{3r^2}{2a_0} e^{-\frac{r}{2a_0}} + \frac{r^3}{4a_0^2} e^{-\frac{r}{2a_0}} \right] \\ &= \frac{1}{a_0} \left[ 2r e^{-\frac{r}{2a_0}} - \frac{2r^2}{a_0} e^{-\frac{r}{2a_0}} + \frac{r^3}{4a_0^2} e^{-\frac{r}{2a_0}} \right] \end{aligned}$$

$$-\frac{\hbar^2}{2m_e} = M, a_0 = \frac{\epsilon_0 \hbar^2}{\pi m_e e^2} \quad (\text{note that } e \text{ is charge of an electron})$$

$$\frac{M}{r^2} \frac{d}{dr} \left[ r^2 \frac{dR(r)}{dr} \right] + \left[ \frac{-2M}{r^2} - \frac{e^2}{4\pi\epsilon_0 r} \right] R(r) = ER(r)$$

$$\frac{M}{r^2} \frac{1}{a_0} \left[ 2r e^{-\frac{r}{2a_0}} - \frac{2r^2}{a_0} e^{-\frac{r}{2a_0}} + \frac{r^3}{4a_0^2} e^{-\frac{r}{2a_0}} \right] + \left[ \frac{-2M}{r^2} - \frac{e^2}{4\pi\epsilon_0 r} \right] \left[ \frac{r}{a_0} e^{-\frac{r}{2a_0}} \right] = E \left[ \frac{r}{a_0} e^{-\frac{r}{2a_0}} \right]$$

$$M \left[ \frac{2}{ra_0} e^{-\frac{r}{2a_0}} - \frac{2}{a_0^2} e^{-\frac{r}{2a_0}} + \frac{r}{4a_0^3} e^{-\frac{r}{2a_0}} \right] - \frac{2M}{ra_0} e^{-\frac{r}{2a_0}} - \frac{e^2}{4\pi\epsilon_0 a_0} e^{-\frac{r}{2a_0}} =$$

$$-\frac{\hbar^2}{2m_e} \left[ -\frac{2\pi m_e e^2}{a_0 \epsilon_0 \hbar^2} e^{-\frac{r}{2a_0}} + \frac{r}{4a_0^3} e^{-\frac{r}{2a_0}} \right] - \frac{e^2}{4\pi\epsilon_0 a_0} e^{-\frac{r}{2a_0}} =$$

$$\left[ \frac{e^2}{4\pi a_0 \epsilon_0} e^{-\frac{r}{2a_0}} - \frac{\hbar^2}{2m_e} \frac{r}{4a_0^3} e^{-\frac{r}{2a_0}} \right] - \frac{e^2}{4\pi\epsilon_0 a_0} e^{-\frac{r}{2a_0}} = -\frac{\hbar^2}{2m_e} \frac{1}{4a_0^2} \left( \frac{r}{a_0} e^{-\frac{r}{2a_0}} \right)$$

$$E = -\frac{\hbar^2}{2m_e} \frac{1}{4a_0^2} = \frac{\hbar^2 \pi m_e e^2}{8m_e a_0 \epsilon_0 \hbar^2} = \frac{\hbar^2 \pi m_e e^2}{32\pi^2 m_e a_0 \epsilon_0 \hbar^2} = \frac{e^2}{32\pi^2 a_0 \epsilon_0}$$

By comparing this energy to  $E_n = -\frac{e^2}{8\pi\epsilon_0 a_0 n^2}$ ,  $n=2$ .

9-4

$$\int_0^\infty r^n e^{-\alpha r} = \frac{n!}{\alpha^{n+1}}$$

$$\langle V \rangle = \frac{1}{\pi a_0^3} \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta \int_0^\infty -\frac{e^2}{4\pi\epsilon_0 r} e^{-\frac{2r}{a_0}} r^2 dr = -\frac{e^2}{4\pi\epsilon_0} \frac{4\pi}{\pi a_0^3} \int_0^\infty r e^{-\frac{2r}{a_0}} dr = -\frac{e^2}{4\pi\epsilon_0 a_0}$$

At ground level,

$$-\frac{e^2}{4\pi\epsilon_0 a_0} = \frac{(1.6 \times 10^{-19})^2}{4 \times 3.14 \times 8.85 \times 10^{-12} \times 5.3 \times 10^{-11}} = 4.345 \times 10^{-18} \text{ J}$$

9-15

$$\psi = R(r)\Theta(\theta)\Phi(\phi)$$

$$\langle z \rangle = \frac{1}{\pi a_0^3} \int_0^{2\pi} d\phi \int_0^\pi \cos\theta \sin\theta d\theta \int_0^\infty r^3 e^{-\frac{2r}{a_0}} dr = \frac{2}{a_0^3} [-\cos^2 \theta]_0^\pi \int_0^\infty r^3 e^{-\frac{2r}{a_0}} dr = 0$$

$$\begin{aligned}\langle z^2 \rangle &= \frac{1}{\pi a_0^3} \int_0^{2\pi} d\phi \int_0^\pi \cos^2 \theta \sin \theta d\theta \int_0^\infty r^4 e^{\frac{-2r}{a_0}} dr = \frac{2}{a_0^3} \left[ -\frac{1}{3} \cos^3 \theta \right]_0^\pi \int_0^\infty r^4 e^{\frac{-2r}{a_0}} dr \\ &= \frac{4}{a_0^3} \int_0^\infty r^4 e^{\frac{-2r}{a_0}} dr = a_0^2\end{aligned}$$

Since H atom is spherically symmetric, values will be the same for the corresponding x and y quantities.

### 9-28

$$\int \int \int \psi_{210} * \psi_{211} = \int \int \int [R(r)\Theta(\theta)\Phi(\phi)]_{210} [R(r)\Theta(\theta)\Phi(\phi)]_{211} d\phi d\theta dr$$

Since the integral over  $\theta$  is zero ( $\int_0^\pi \cos \theta \sin^2 \theta d\theta = 0$ ), they are orthogonal.