CHEM 1410 HW # 6
P9.4, 9.6, 9.11, 18, 24
Due Oct. 27, 2008

9.4

$$\iiint \psi_{210}^{*}(\tau)\psi_{211}(\tau)d\tau = \frac{1}{\sqrt{32}\sqrt{64}\,\pi\, a_0^3}\int_0^{2\pi} e^{+i\phi}d\phi \int_0^{\pi}\cos\theta\sin^2\theta\, d\theta \int_0^{\infty}\left(\frac{r}{a_0}\right)^2 e^{-r/a_0}dr$$

This integral is zero because $\int_0^{\pi}\cos\theta\sin^2\theta\, d\theta = \left[\frac{\sin^3\theta}{3}\right]_0^{\pi} = 0-0=0.$

It is sufficient to evaluate the integral over θ.

9.6

The functions have n–l–1 radial nodes and l angular nodes. Therefore

a) $\psi_{2p_x}(r,\theta,\phi)$ has no radial nodes and one angular node.

b) $\psi_{2s}(r)$ has one radial node and no angular nodes.

c) $\psi_{3d_{xz}}(r,\theta,\phi)$ has no radial nodes and 2 angular nodes.

d) $\psi_{3d_{x^2-y^2}}(r,\theta,\phi)$ has no radial nodes and 2 angular nodes.

9.11

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

$$\langle r\rangle = \frac{4}{a_0^3}\int_0^{\infty} r^3 e^{-\frac{2r}{a_0}} dr$$

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

$$\langle r\rangle = \frac{4}{a_0^3}\frac{6a_0^4}{16} = \frac{3}{2}a_0$$

9.18

$$\langle E_{kinetic}\rangle = \int \psi^*(\tau)\hat{E}_{kinetic}\psi(\tau)d\tau$$

$$\langle E_{kinetic}\rangle = -\frac{\hbar^2}{2m_e}\frac{1}{\pi a_0^3}\int_0^{2\pi} d\phi\int_0^{\pi}\sin\theta\, d\theta\int_0^{\infty} e^{-r/a_0}\left(\frac{1}{r^2}\frac{d}{dr}\left[r^2\frac{d}{dr}e^{-r/a_0}\right]\right)r^2 dr$$

$$\langle E_{kinetic}\rangle = -\frac{\hbar^2}{2m_e}\frac{4}{a_0^3}\int_0^{\infty}\left[-\frac{2r}{a_0}e^{-2r/a_0} + \frac{r^2}{a_0^2}e^{-2r/a_0}\right]dr = \frac{\hbar^2}{m_e}\frac{4}{a_0^4}\int_0^{\infty} r e^{-2r/a_0}dr - \frac{\hbar^2}{m_e}\frac{2}{a_0^5}\int_0^{\infty} r^2 e^{-2r/a_0}dr$$

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

$$\langle E_{kinetic}\rangle = \frac{\hbar^2}{m_e}\frac{4}{a_0^4}\frac{a_0^2}{4} - \frac{\hbar^2}{m_e}\frac{2}{a_0^5}\frac{2a_0^3}{8} = \frac{\hbar^2}{2m_e a_0^2} = \frac{\hbar^2\pi m_e e^2}{2m_e a_0\varepsilon_0 h^2} = \frac{e^2}{8\pi a_0\varepsilon_0}$$

$$\left\langle E_{potential} \right\rangle = \int \psi^*(\tau) \hat{E}_{potential} \psi(\tau)\, d\tau$$

$$\left\langle E_{potential} \right\rangle = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{\pi a_0^3}\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta \int_0^{\infty} \left[e^{-r/a_0}\right]\left(\frac{1}{r}\right)\left[e^{-r/a_0}\right] r^2 dr$$

$$\left\langle E_{potential} \right\rangle = -\frac{e^2}{4\pi\varepsilon_0}\frac{4}{a_0^3}\int_0^{\infty} r\, e^{-2r/a_0} dr = -\frac{e^2}{4\pi\varepsilon_0}\frac{4}{a_0^3}\frac{a_0^2}{4} = -\frac{e^2}{4\pi\varepsilon_0 a_0}$$

9.24

$$\langle r \rangle_{nl} = \frac{n^2 a_0}{Z}\left[1 + \frac{1}{2}\left(1 - \frac{l(l+1)}{n^2}\right)\right]$$

$$n = \sqrt{\frac{2Z \times \langle r \rangle_{n0}}{3a_0}} = \sqrt{\frac{2000a_0}{3a_0}} = 25.82 \approx 26$$

$$I = \frac{Z^2 e^2}{8\pi\varepsilon_0 a_0 n^2} = \frac{\frac{Z^2}{n^2} \times \left(1.602 \times 10^{-19}\mathrm{C}\right)^2}{8\pi \times 8.854 \times 10^{-12}\mathrm{J^{-1}C^2m^{-1}} \times 5.292 \times 10^{-11}\mathrm{m}} \times \frac{1\,\mathrm{eV}}{1.602 \times 10^{-19}\mathrm{J}}$$

$$I = 13.6039\frac{Z^2}{n^2}\,\mathrm{eV} = 13.6039\frac{1}{n^2}\,\mathrm{eV} \quad \text{for the H atom.}$$

For the ground state, $I = 13.6039$ eV and for $n = 26$, $I = 0.0201$ eV.