Chemistry 163A

Problems

28. Describe

(a) The mathematical origins of the n, ℓ, m_ℓ quantum numbers for the hydrogen atom.

(b) The physical significance of the n, ℓ, m_ℓ, m_s quantum numbers for the hydrogen atom.

29. McQ. #6-34. (2s, 2p required; 3s is optional *)

30. McQ. #6-30

[*required part:* set up appropriate integral for P(R), the probability electron is within distance R of nucleus; **optional part*: evaluate integral and find $R_{50\%}$ and $R_{90\%}$ solving resulting equation by "table" or "graphically"]

31. Which are eigenfunctions? For those that are eigenfunctions, what are the eigenvalues?

(a) $\hat{\ell}^2\psi_{2px}$ *(b) $\hat{\ell}^2\psi_{3dxy}$

(c) $\hat{\ell}_z\psi_{2px}$ *(d) $\hat{\ell}_z\psi_{2py}$

*(e) $\hat{\ell}_z(\psi_{2px} + i\psi_{2py})$

*(f) What do the (correct) results for parts (d) and (e) say about the properties of the real and complex 2p orbitals?

32. Using the normalized trial function

$$\psi_{trial} = \left(\frac{\alpha^3}{\pi}\right)^{1/2} e^{-\alpha r} \text{ and}$$

the hamiltonian for the hydrogen atom (in atomic units):

$$H_{op} = \left\{-\frac{1}{2}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] - \frac{Z}{r}\right\}$$

i) Apply the variation method to get the best value of α.

ii) What is $\langle E\rangle$ for this value of α?

iii) Comment (intelligently) on the values of $\langle E\rangle$ and α.

*33. McQ #8-17.

34. Why do the ^1S and ^3S (1s 2s) excited states of the helium have different energies? Which is lower?

35. Assuming the energy of the outermost electron in an atom is given by the hydrogen energy with an effective nuclear charge Z_f, use the following ionization potentials (IP) and electron affinities (EA) to determine Z_f and an effective radius r_f (use Bohr radius) for the following atoms and ions: Li, Li^-, Be, N, O, O^-, F, F^-, Ne, Na, Mg, S, S^-, Cl, and Cl^-.

	Li	Be	N	O	F	Ne	Na	Mg	S	Cl
IP (ev)	5.30	9.32	14.54	13.61	17.42	21.56	5.14	7.64	10.36	13.01
Ea (ev)	.62			1.47	3.40		.54		2.07	3.61