Chemical Physics Cumulative Exam
Monday September 26, 2005

1.(20 points) Consider a hydrogen atom with the nucleus at the origin and the electron in a $|2p_z\rangle$ state.

a. Derive an expression for the *zz* component of the atomic quadrupole moment. The quadrupole operator is $-Ar^2Y_2^0(\theta,\phi)$ where *A* is a constant. Simplify the result as much as you can (do the integrations).

b. Derive an expression for the *zz* component of the electric field gradient at the nucleus. The electric field gradient operator is $\frac{B}{r^3}Y_2^0(\theta,\phi)$ where *B* is a constant. Simplify the result as much as you can (do the integrations).

2. (30 points) Consider the *HF* molecule in its ground state.

a. How would you measure its dipole moment?

b. How would you calculate its dipole moment?

c. Sketch the anticipated dipole moment as a function of bond length.

3. (10 points) How would you calculate the dipole polarizability of the H atom in its ground state?

4. (20 points) Identify which of the following molecules is paramagnetic and explain your answer.

a. O_2
b. *ON*
c. N_2
d. *HOO*
e. *HNO*

5. (20 points) The spin Hamiltonian for the H atom in its ground state has the form
$\hat{H} = g_e\beta_e H\hat{S}_z + g_N\beta_N H\hat{I}_z + a\hat{I}\bullet\hat{S}$

a. Identify the terms.
b. Calculate, to first order, the energy levels of this system.

Useful equations

$$\left|2p_z\right\rangle = \sqrt{\frac{1}{24a_0^5}} r \exp(-\frac{r}{2a_0}) Y_1^0(\theta,\phi)$$

$$Y_1^0(\theta,\phi) Y_1^0(\theta,\phi) = \frac{1}{\sqrt{5\pi}} Y_2^0(\theta,\phi) + \frac{1}{\sqrt{4\pi}} Y_0^0(\theta,\phi)$$

$$\int_0^\infty x^N e^{-ax} dx = \frac{N!}{a^{N+1}}$$

$$\int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \; Y_{l_1}^{m_1^*}(\theta,\phi) Y_{l_2}^{m_2}(\theta,\phi) = \delta_{l_1 l_2} \delta_{m_1 m_2}$$

$$\hat{S}_x \alpha = \frac{\beta}{2} \quad ; \quad \hat{S}_x \beta = \frac{\alpha}{2}$$

$$\hat{S}_y \alpha = \frac{i\beta}{2} \quad ; \quad \hat{S}_y \beta = \frac{-i\alpha}{2}$$