Homework 9, Due April 8

1. Establish the conversion factors between the following energy units: eV, kcal/mol, Hartree, cm^{-1}, and J.

2. Prove using relevant spin operators that the following spin wave function corresponds to the M_s=0 component of the triplet excited state of He:

$$\left|\alpha(1)\right\rangle\left|\beta(2)\right\rangle + \left|\beta(1)\right\rangle\left|\alpha(2)\right\rangle$$

3. Write the Slater determinant for the ground state of Be.

4. In the matrix representation of the spin, the eigenfunctions are given as

$$|\alpha\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad |\beta\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and the three components of the spin angular momentum are given as

$$\hat{s}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \hat{s}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \hat{s}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

   a. Show that $|\alpha\rangle$ and $|\beta\rangle$ are indeed the eigenfunctions of $\hat{s}_z$ and $\hat{s}^2$.
   b. Prove the commutation relation $[\hat{s}_x, \hat{s}_y] = i\hbar\hat{s}_z$.
   c. Construct the matrix representations for $\hat{s}_+$ and $\hat{s}_-$, and show that their actions on an eigenfunction yield either 0 or the other eigenfunction.