

HW #9 Chem 2430

1. Write the wave function including spin of the $M_L=2$ component of the 1D state of C ($1s^2 2s^2 2p^2$) (You can ignore the $1s^2 2s^2$ electrons.)

Can this wave function be represented as a single Slater determinant when using orbitals that are eigenfunctions of \hat{L} and \hat{m}_L ?

Write this wave function in terms of P_x, P_y, P_z .

2. What are the states, including J values, that result from a pd electronic configuration?
3. For the He atom show that the configuration $1s^2 (\alpha\beta - \beta\alpha)$ does not mix directly with $(1s2s + 2s1s)(\alpha\beta - \beta\alpha)$.
4. Show that p and p^5 give the same electronic states. Also show that p^2 and p^4 give the same electronic states.
5. In a restricted Hartree-Fock calculation on Li the wave function is $|1s \bar{1s} 2s|$, where the spatial parts of the $1s\alpha$ and $1s\beta$ orbitals are the same.

In the unrestricted Hartree-Fock (UHF) approximation, the wave function is $|1s' \bar{1s}'' 2s'|$ where the $1s\alpha$ and $1s\beta$ orbitals have different spatial parts. Assume that you have only two basis functions χ_1 and χ_2 that are of the form $e^{-\alpha r}$. Show that the UHF wave function is multiconfigurational when re-expressed in terms of the orbitals of the restricted Hartree-Fock wave function.