CHEMISTRY 3BB3 1999/2000

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ASSIGNMENT 8

DUE: April 6, 2000

1. A student has given you the table below, for the molecular orbitals of formaldehyde. The MO's are represented as columns, with the energy at the top. The coefficients of each of the atomic orbitals are given by the elements down the column. Sketch each of the occupied orbitals, and label it properly according to the group theory designation.

Energy	44.2	20.1	19.2	-9.8	-13.8	-15.2	-15.4	-16.6	-22.1	-34.7
C 2S	-0.744	0.065	0.000	0.000	0.000	0.000	0.000	0.000	-0.642	0.337
C Py	0.000	0.000	0.683	0.000	-0.262	0.000	0.000	-0.559	0.000	0.000
C Px	0.000	0.000	0.000	0.871	0.000	0.000	0.371	0.000	0.000	0.000
C Pz	-0.043	-0.719	0.000	0.000	0.000	-0.268	0.000	0.000	0.348	0.152
H 1S	0.401	-0.314	-0.509	0.000	-0.304	0.166	0.000	-0.398	-0.328	0.027
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O 2S	0.268	0.428	0.000	0.000	0.000	0.143	0.000	0.000	0.414	0.927
O Py	0.000	0.000	-0.120	0.000	0.864	0.000	0.000	-0.609	0.000	0.000
O Px	0.000	0.000	0.000	-0.491	0.000	0.000	0.929	0.000	0.000	0.000
O Pz	-0.226	-0.313	0.000	0.000	0.000	0.923	0.000	0.000	0.281	0.042

2. Is the LUMO a π or a σ orbital? Is it bonding (π, σ) or antibonding (π^*, σ^*) ? Explain briefly.

3. For the following partial electronic configurations, list the possible electronic states (including spin multiplicity). Any unspecified orbitals are filled. Make sure you use the proper group-theoretical symbols. The table in the back of Harris on direct products of group representations will be useful.

a) water: $(a_1)^2(a_1)^1(b_1)^1$

b) water: $(a_1)^2(b_2)^1(b_1)^1$

c) square planar complex: $(b_{2g})^1(b_{1g})^1$

d) square planar complex: $(e_g)^2$ (optional, for bonus marks)

4. The triplet combination, with z component of +1, of two spins (1/2) is given by $\alpha\alpha$, where α is the wavefunction of a single spin with total angular momentum of 1/2 and a z component of +1/2. Show that this is an eigenfunction (with the correct eigenvalue) of the total angular momentum operator, L^2, which is equal to $(I+J)^2$, where I and J are the individual angular momentum operators.

Hint: Remember that $(I+J)^2$ is the dot product of $(I+J)$ with itself and

$$I \cdot I = I_x^2 + I_y^2 + I_z^2 = 1/2\left(I_+ I_- + I_- I_+\right) + I_z^2$$