Symmetry and Group Theory – Exercise Set 5

5.1) Show that the nitrogen p_x and p_y orbitals in NH_3 form the basis for an irreducible representation of C_{3v}.

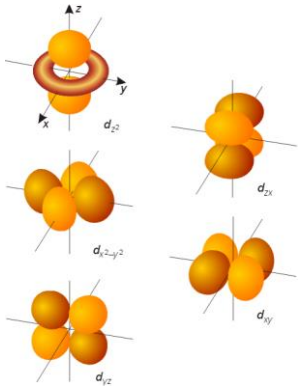
5.2) The characters $\chi(R)$ of the representation of a direct product are the products of the characters $\chi_1(R)$ and $\chi_2(R)$ of the representations for which the individual functions are the basis, *i.e.* $\chi(R) = \chi_1(R)\chi_2(R)$. Demonstrate this for one-dimensional (irreducible) representations, where the proof is particularly simple.

5.3) In the C_{3v} point group, what are the characters of the representation belonging to the direct products $A_1 \otimes A_1$, $A_1 \otimes A_2$, $A_2 \otimes E$, $E \otimes E$, and $E \otimes E \otimes E$? Which irreducible representations are contained?

5.4) Determine the symmetry species (the irreducible representation(s)) of the carbon p orbitals in CH_4.

5.5) Determine the symmetry species (the irreducible presentation(s)) of the four hydrogen 1s orbitals in CH_4.

5.6) In the context of crystal or ligand field theory, we frequently deal with the symmetry of the metal orbitals. For a square planar complex ML_4, determine the irreducible representations of the metal s, p, and d orbitals. In this case, this can still be easily done by visual inspection. The shape of the d orbitals is sketched to the right.

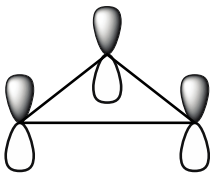


5.7) Construct the qualitative MO diagram of CH_3^+ (trigonal planar).

Homework

5.8) In the cyclopropenyl cation ($C_3H_3^+$), the three carbon atoms form an equilateral triangle. One can use the three carbon $2p_z$ orbitals to construct the molecular π orbitals of the cyclopropenyl cation.

a) Determine the symmetry species of these molecular π orbitals.
b) Draw a qualitative MO diagram for these π orbitals. In other words, draw an energy diagram showing how the three p orbitals split up to form the molecular orbitals.
c) Write down the Symmetry Adapted Linear Combinations (SALCs) of these π orbitals (neglect normalization). Hint: You can figure the coefficients of the SALCs out by considering the shape of atomic orbitals of the same symmetry species.



5.9) A molecule AB_6 has a trigonal prismatic structure. Assume that the orbitals of atom A that are involved in bonding are the 2s orbital and the three 2p orbitals. For the atoms B, assume that each bond is with an s orbital.

a) Determine the symmetry species of all orbitals.
b) Draw a qualitative MO diagram. The exact energy ordering of the MOs is not important.