

Applications of Group Theory

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Lectures

Exercises

9.2.01, Mondays, 14:15

7.1.21, Fridays, 10:15

Sheet 8

1. Molecular stability

Why would the octahedral configuration of Fig. 1b be more stable for a hypothetical SH_6 than the planar configuration in Fig. 1a? Consider the angular momentum states required for the S atom to make the appropriated equivalent valence bonds to the six hydrogens in the planar SH_6 hypothetical molecule.

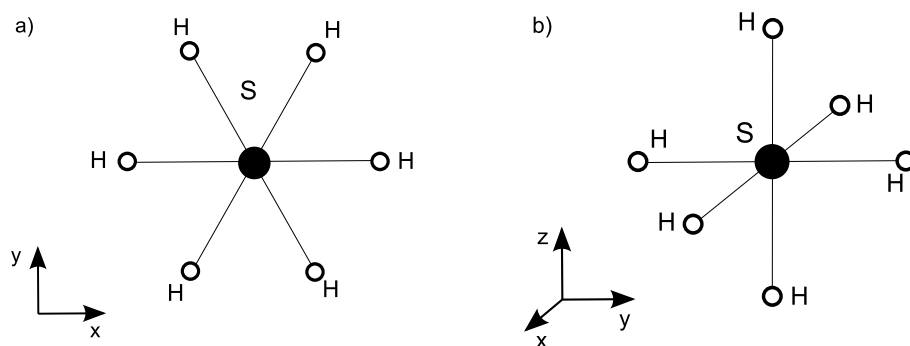


Figure 1: Two possible configurations of the hypothetical molecule SH_6 .

2. Ethylene

Ethylene (C_2H_4) is a planar molecule which has the configuration shown in Fig. 2.

1. Identify the appropriate point group for C_2H_4 .
2. Find the equivalence representation for the two carbon atoms and the four hydrogen atoms in the ethylene molecule.
3. Considering the directed valence orbitals (generalization of the equivalent bond orbitals) how do the carbon atoms satisfy their bonding requirements? Which angular momentum states are needed to form bonding orbitals from each carbon atom?
4. Give the block diagonal structure for the secular equation of the electronic energy levels of ethylene (reduce yourself to the valence orbitals of the constituent atoms).

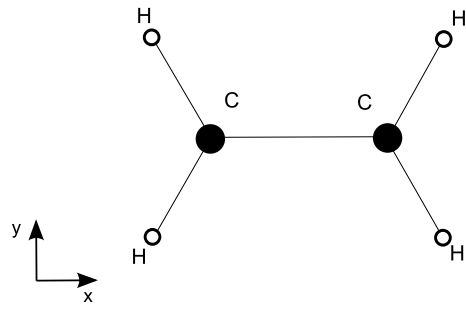


Figure 2: Geometrical configuration of ethylene (C₂H₄).

Frohes Schaffen!