University of Regensburg Summer Term 2016

Applications of Group Theory

PD Dr. Andrea Donarini

Lectures H33, Mondays, 14:15
5.0.21, Wednesdays, 13:15

Exercises H34, Thursdays, 14:15

Sheet 7

1. Methane

Consider the methane molecule CH_4. We want to study the nature of the chemical bonding of the carbon with the four hydrogen atoms.

1. Consider the Hilbert space generated by the four 1s orbitals of the hydrogen atoms contained in a methane molecule. Construct the character system for the associated representation relative to the point group of methane. Find the irreducible representations contained in it.
2. Now consider the electronic structure of the carbon atom, $1s^2 2s^2 2p^2$, and restrict yourself to the valence orbitals. Determine the hybridization of the carbon atom compatible with the irreducible representations obtained at point 2).
3. Using symmetry arguments construct the molecular orbitals of methane as linear combination of carbon and hydrogen atomic orbitals. Hint: Do not try to obtain the exact orbitals. Limit yourself to the symmetry and the bonding/antibonding character of the orbitals.
4. Give an explicit expression for the equivalent bond orbitals of methane in terms of the valence atomic orbitals of the carbon atom.

2. 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.

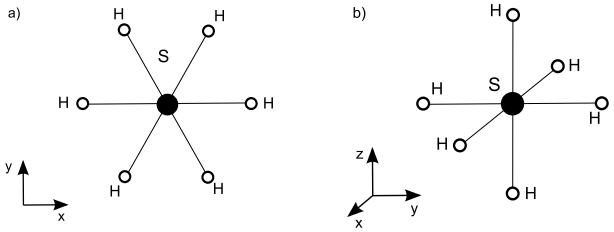

Figure 1: Two possible configurations of the hypothetical molecule SH_6.

Frohes Schaffen!