Applications of Group Theory

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Lectures   9.2.01, Mondays, 14:15
Exercises   H34, Wednesdays, 14:00

Sheet 8

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. Which is the point group of methane? Its character table?

2. Consider the Hilbert space generated by the four 1s orbitals of the hydrogen atoms. Construct the character system for the associated representation relative to the point group of methane. Find the irreducible representations contained in it.

3. 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). Hint: It is useful to consider the basis functions associated to the irreducible representations and compare their symmetry with the one of the valence atomic orbitals of C.

4. 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 numbers. Limit yourself to the symmetry and the bonding/antibonding character of the orbitals.

5. Give an explicit expression for the equivalent bond orbitals of methane in terms of the valence atomic orbitals of its constituents.

Frohes Schaffen!