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Study Notes on Huckel Molecular Orbital Theory

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Huckel Molecular Orbital Theory

In conjugated systems, the Hückel approximation is used to derive the energies and forms of the π molecular orbitals. The covalent bonding in these hydrocarbons may be divided into two different "frameworks" using the Hückel approximation: the σ -bonding framework and the π -bonding framework. Different combinations of atomic orbitals produce the wavefunctions used to characterise the bonding orbitals in each framework.

The approach is limited to conjugated hydrocarbons, and only π electron molecular orbitals are taken into account because they govern the general features of these compounds; sigma electrons are omitted. The orthogonality of and orbitals in planar molecules justifies this phenomenon, which is known as sigma-pi separability. As a result, the Hückel approach is only applicable to planar systems.

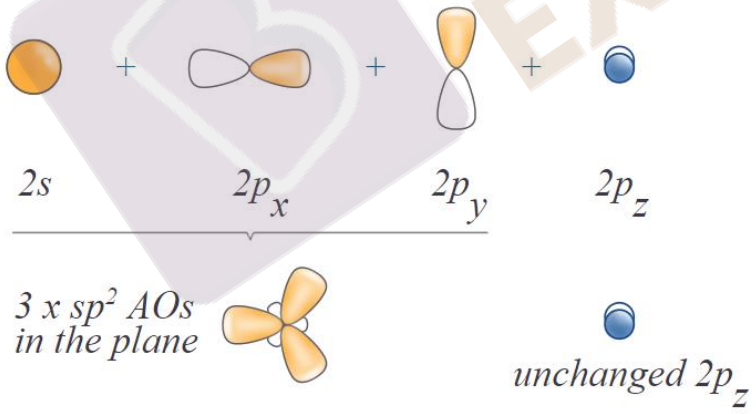
The Hückel approximation assumes that the electrons in the π bonds "experience" an electric potential due to the complete
σ -bonding framework in the molecule (i.e., it concentrates solely on bond creation because the σ bonding framework has already been constructed).

Conjugated System

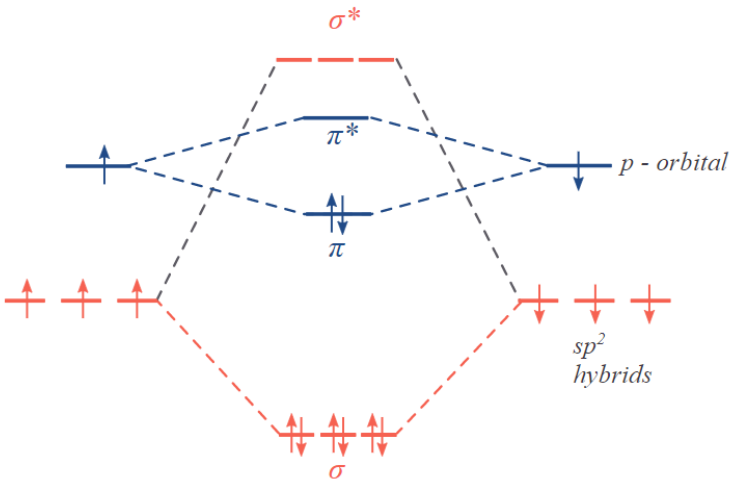
A conjugated system has an area of overlapping p-orbitals that spans the interjacent single bonds and allows electrons to delocalize across all of the aligned p-orbitals. These π electrons belong to a group of atoms rather than a single bond or atom.

Ethylene

Before considering the Hückel treatment for ethylene, it's a good idea to analyse the molecule's overall bonding image. In ethylene, bonding occurs when the 2s, 2px, and 2py atomic orbitals on each carbon atom are sp^2 hybridised, leaving the 2pz orbitals unaffected.



The σ-bonding framework is formed by the mixing of electrons in the sp^2 hybrid orbitals on carbon and the electrons in the 1s atomic orbitals of the four hydrogen atoms. The unhybridized 2pz orbitals give rise to the -π bonding framework. The resulting molecular orbital diagram demonstrates the independence of these two frameworks.



The HMO theory is an approximation method for treating planar conjugated hydrocarbons that simplifies the variation method.

- This theory distinguishes between σ electrons and π electrons.
- π -electrons play a major role in determining the properties of conjugated compounds.
- The variation approach and the LCAO(π)-MO approximation are used to calculate HMO.

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