Molecular orbital and valence-bond theory

Bonding in benzene

Conjugation in $\pi$-Systems: Valence-Bond Benzene
Conjugation in $\pi$-Systems:
Valence-Bond Benzene
Failure of the qualitative VB model

- Benzene is stable
- Cyclobutadiene is unstable
  - Why should this be so??
Conjugation in $\pi$-Systems:
Molecular Orbitals of Benzene and Hexatriene

The quick brown fox jumped over the lazy dog.

Conjugation in $\pi$-Systems:
Molecular Orbitals of Benzene
Conjugation in $\pi$-Systems:
Molecular Orbitals of Cyclobutadiene

Conjugation in $\pi$-Systems:
Benzene and Hückel’s Rule

Six uncombined $2p$ orbitals, each with one electron

In the ground-state electron configuration of benzene, all six electrons are in pi bonding MOs
Frost circles for 4-, 5-, and 6-membered rings

Origin of the 4n+2 \(\pi\)-electrons in pyridine

This orbital is perpendicular to the six 2\(\text{p}\) orbitals of the pi system.

This electron pair is not a part of the 4\(n\) + 2 pi electrons.
Origin of the $4n+2$ $\pi$-electrons in furan and pyrrole

This electron pair is a part of the $4n + 2$ pi electrons.

This electron pair is not a part of the $4n + 2$ pi electrons.

Compare geometries: pyrrole and pyrrolidine