

Answers to Exercise 5.3

Valence Bond Theory vs. Molecular Orbital Theory

1. Valence bond theory treats electrons as localized between pairs of atoms. So, each electron is considered to belong to just one bond, and each bond only involves two atoms.
Molecular orbital theory treats electrons as delocalized across the whole molecule. So, each electron is considered to reside in one molecular orbital, but that molecular orbital may be spread across many (or all) of the atoms in the molecule.
2. In molecular orbital theory, atomic orbitals on **different** atoms are combined to make molecular orbitals.
In valence bond theory, atomic orbitals on **the same** atom are combined to make hybrid atomic orbitals.
3.
 - (a) A set of two sp orbitals is formed by hybridizing an s orbital and a p_z orbital.
 - (b) A set of three sp^2 orbitals is formed by hybridizing an s orbital, a p_x orbital and a p_y orbital.
 - (c) A set of four sp^3 orbitals is formed by hybridizing an s orbital, a p_x orbital, a p_y orbital, and a p_z orbital.

The convention of dividing the p orbitals such that the p_x and p_y orbitals have the same symmetry while the p_z orbital has the other kind of symmetry is used in both molecular orbital theory and valence bond theory.

Since hybridized orbitals are always sigma symmetric (and the unhybridized p orbitals are pi symmetric), if two p orbitals are required to make the hybrid orbitals, they will be p_x and p_y . If only one p orbital is required to make the hybrid orbitals, it will be p_z .