

VSEPR Theory and VB Theory

VSEPR

Valence Shell Electron Pair Repulsion

The various electron regions (both bonding and non-bonding) surrounding an atom will have great repulsive forces upon one another.

These repulsions will force a specific three dimensional geometry surrounding the central atom. The final shape is the shape where the repulsive forces are minimized.

What are **electron regions**? These are the regions or zones where the electrons “hang out” around the central atom. You will need to count how many “groupings” of electrons there are. Each of the following is considered ONE electron region...

single bond

double bond

triple bond

lone pair

Our textbook refers to these electron regions as “effective electron pairs” (p. 639).

Electronic Geometry

This is the three dimensional shape around the central atom of the ELECTRON REGIONS.

There are only 5 possible electronic geometries.

Molecular Geometry

This is the three dimensional shape around the central atom of the ATOMS. There are at least 12 possible shapes and names here.

Molecular geometries are BUILT on top of electronic geometries. The reason for more shapes (and names) is because lone pair electrons are NOT part of the molecular shape. As you introduce more lone pairs to a shape, you will get new shapes with new names.

Valence Bond (VB) Theory

Why even have VB theory when VSEPR theory seems to cover all the shapes and angles that we need? The following points are made...

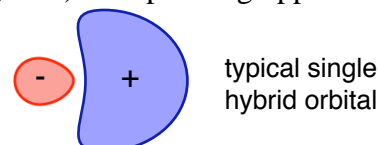
- VSEPR addresses SHAPES only - the logic is based solely on repulsions of negative regions.
- VB Theory actually addresses the BONDING that must occur. Bonding from the OVERLAP of atomic orbitals.
- Both theories have their merits
- Both theories work well in a cooperative way (learn them both!)

Hybrid Orbitals

Hybridization of orbitals is a key component of VB theory. A hybrid orbital is really just a mathematical combination of atomic orbital wavefunctions. The atomic wavefunctions (ψ 's) are combined in such a way that we get new orbitals that actually have the exact geometry as predicted by VSEPR theory. These new orbitals are called hybrids. We have as many hybrid orbital sets as we have electronic geometries - five.

Keep these things in Mind for VB Theory

- The same filling rules still apply. Only 2 electrons max per orbital and electrons occupy levels singly before pairing begins.
- Each hybrid we make will be part of a SET of hybrid orbitals - these SETS will have the same geometries of our 5 electronic geometries that VSEPR theory predicted.
- You will always get as many hybrid-orbitals as you do atomic orbitals to make them.
- Generally speaking, all hybrid orbitals have the same basic shape - a large positive lobe pointing one direction and another (smaller and negative) lobe pointing opposite (180°).



- All the hybrid orbitals in a SET are degenerate.
- It is the OVERLAP of orbitals that leads to bonding. In wave-theory, this is called constructive interference.

Our “Quick and Dirty” Method for Drawing Hybrid Orbital Sets

We generally do not want to take the time to draw both ends of those hybrid orbitals - afterall, it is the larger positive end that we are generally interested in for bonding overlap. Plus, we also don't like showing the “fatness” of that lobe out there. So here's what is typically drawn...



Note that this is the tetrahedral set of four sp^3 hybrids. Each of the five electronic geometries has a corresponding set of hybrid orbitals. Refer to the other help sheet on electronic and molecular geometries for the pictures and names.