

Finding Bond Angles, Shapes, and Hybridizations

Gettin' funky, VSEPR style

<http://misterguch.brinkster.net/VSEPR.html>

Sometimes people have a hard time with the whole VSEPR thing. In this helpdesk section we'll discuss what VSEPR means, what it's all about, and how you can use a great big flow chart to figure out the bond angles, shapes, and hybridizations of various covalent compounds.

What is VSEPR?

VSEPR stands for Valence Shell Electron Pair Repulsion. It's a complicated acronym, but it means something that's not difficult to understand. Basically, the idea is that covalent bonds and lone pair electrons like to stay as far apart from each other as possible under all conditions. This is because covalent bonds consist of electrons, and electrons don't like to hang around next to each other much because they have the same charge.

This VSEPR thing explains why molecules have their shapes. If carbon has four atoms stuck to it (as in methane), these four atoms want to get as far away from each other as they can. This isn't because the atoms necessarily hate each other, it's because the electrons in the bonds hate each other. That's the idea behind VSEPR.

What is hybridization?

Now, one problem with the whole VSEPR thing is that if you have four things stuck to carbon, for example, there are no orbitals that want to get 109.5 degrees apart from each other (109.5 degrees corresponds to the geometric maximum distance the atoms can get apart). After all, s-orbitals go in a complete sphere (360 degrees) and p-orbitals are 90 degrees apart.

What happens instead of using s- or p- orbitals is that when covalent bonds are formed, the s- and p-orbitals mix to form something called hybrid orbitals. "Hybrid" just means "mixture of two different things", and that's exactly what a hybrid orbital is. When three p-orbitals with 90 degree angles combine with one s-orbital with 360 degrees, they average to form four sp^3 orbitals with 109.5 degree bond angles. Depending on the numbers of s- and p-orbitals that mix, you can get a bunch of different bond angles.

Common shapes you should know

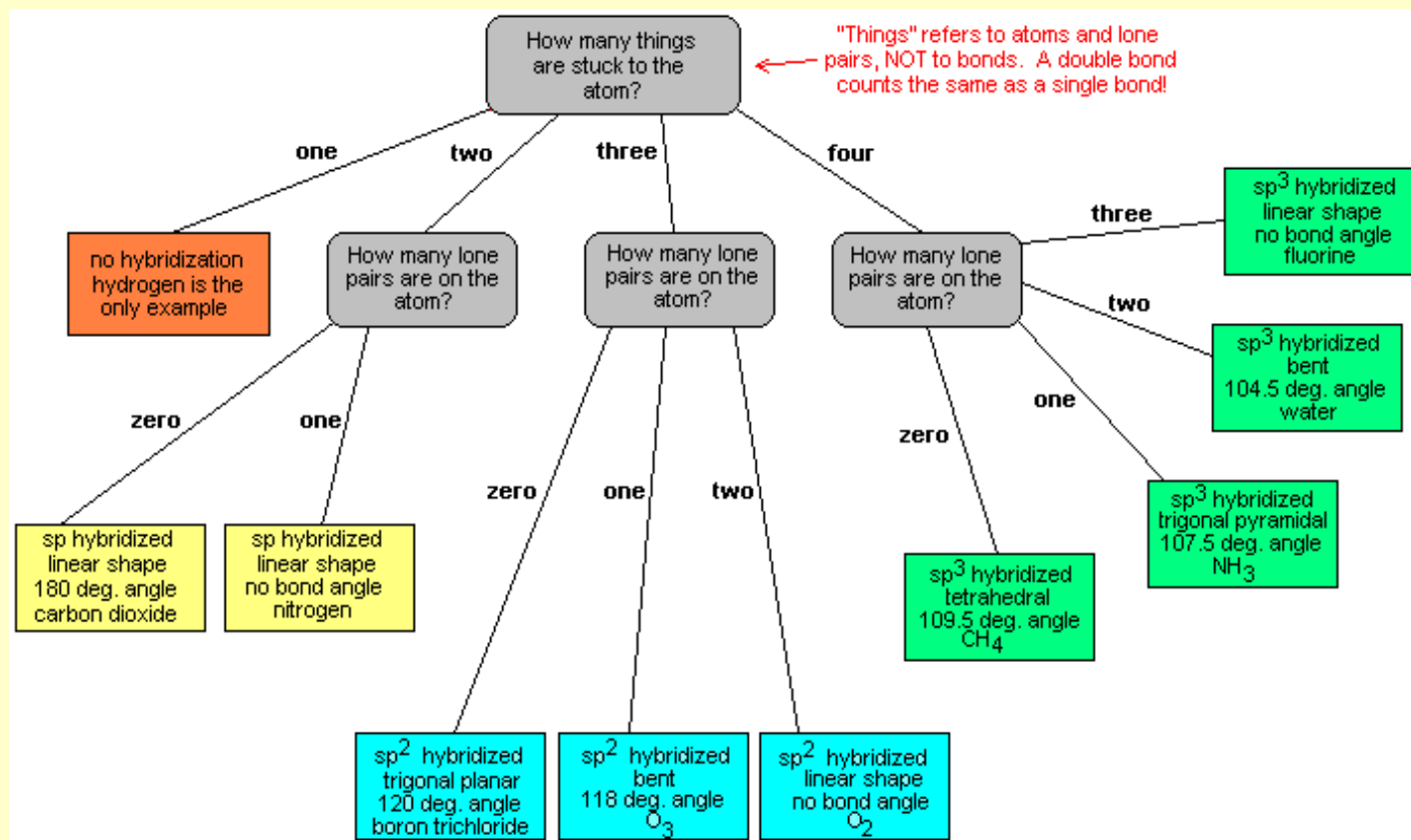
There are a whole bunch of common shapes you need to know to accurately think of covalent molecules. Here they are:

- **Tetrahedral:** Tetrahedral molecules look like pyramids with four faces. Each point on the pyramid corresponds to an atom that's attached to the central atom. Bond angles are 109.5 degrees.
- **Trigonal pyramidal:** It's like a tetrahedral molecule, except flatter. It looks kind of like a squished pyramid because one of the atoms in the pyramid is replaced with a lone pair. Bond angles are 107.5 degrees (it's less than tetrahedral molecules because the lone pair shoves the other atoms closer to each other).
- **Trigonal planar:** It looks like the hood ornament of a Mercedes automobile, or like a peace sign with that bottom-most line gone. The bond angles are 120 degrees.
- **Bent:** They look, well, bent. Bond angles can be either 118 degrees for molecules with one lone pair or 104.5 degrees for molecules with two lone pairs.

- **Linear:** The atoms in the molecule are in a straight line. This can be either because there are only two atoms in the molecule (in which case there is no bond angle, as there need to be three atoms to get a bond angle) or because the three atoms are lined up in a straight line (corresponding to a 180 degree bond angle).
- **There are other types, but we won't worry about them.**

Using a flow chart to figure out what hybridization, shape, and bond angle an atom has

Take a look at this flow chart. I'll explain how to use it to find all the stuff above at the end.



Complicated, huh? Here's how to use it:

- 1) **Draw the Lewis structure for the molecule.** This vital if you're going to get the answer right.
- 2) **Count the number of "things" on the atom you're interested in.** Let's say that you're looking at methane, CH₄. If you want to find the bond angles, shape, and hybridization for carbon, count the number of things that are stuck to it.

Now, the vague term "things" refers to atoms and lone pairs. IT DOES NOT REFER TO THE NUMBER OF BONDS! When you look at methane, there are four atoms stuck to it, so you'd go down the line that says "four" toward the green boxes on this chart.

People get confused with multiple bonds. Take carbon dioxide, for example. There are four bonds (carbon is double-bonded to each oxygen) but only two oxygen atoms bonded to carbon. In this case, we count two things stuck to carbon, because we only count the atoms, NOT the number of

bonds.

Likewise, with ammonia there are four things. Three of the things on nitrogen are hydrogen atoms and the fourth is a lone pair. For the purposes of VSEPR, lone pairs count exactly the same as atoms, because they consist of negative charge, too.

3) Count the number of lone pairs that are on the atom you're interested in. IMPORTANT: This does NOT mean to count the number of lone pairs on all of the atoms in the molecule. Lone pairs on other atoms aren't important - what's important is only what's directly stuck to the atom you're interested in.

We mentioned above that methane has four things stuck to it. Since all four things are hydrogen atoms, we moved toward the green boxes on the flow chart. When we get to our second question, we find that there are no lone pairs on carbon, so our answer is zero. When we go down the line that says "zero" from that box, we find that methane is sp^3 hybridized, with a 109.5 degree bond angle and tetrahedral shape.

And, hey, that's what we were looking for!

Some sample problems:

What are the shapes, bond angles, and hybridizations of the following molecules? Use the flow chart and instructions above to figure it out.

- 1) carbon tetrabromide
- 2) phosphorus trichloride
- 3) oxygen
- 4) the chlorine atom in hydrochloric acid (HCl)
- 5) boron trichloride
- 6) CH_2O
- 7) sulfur difluoride
- 8) either carbon atom in C_2H_2

The answers are below:

- 1) sp^3 , tetrahedral, 109.5 degrees.
- 2) sp^3 , trigonal pyramidal, 107.5 degrees.
- 3) sp^2 , linear, no bond angle
- 4) sp^3 , linear, no bond angle
- 5) sp^2 , trigonal planar, 120 degrees
- 6) sp^2 , trigonal planar, 120 degrees
- 7) sp^3 , bent, 104.5 degrees
- 8) sp , linear, 180 degrees