

Hybrid Orbitals

Skills to Develop

- Describe how to construct hybrid orbitals

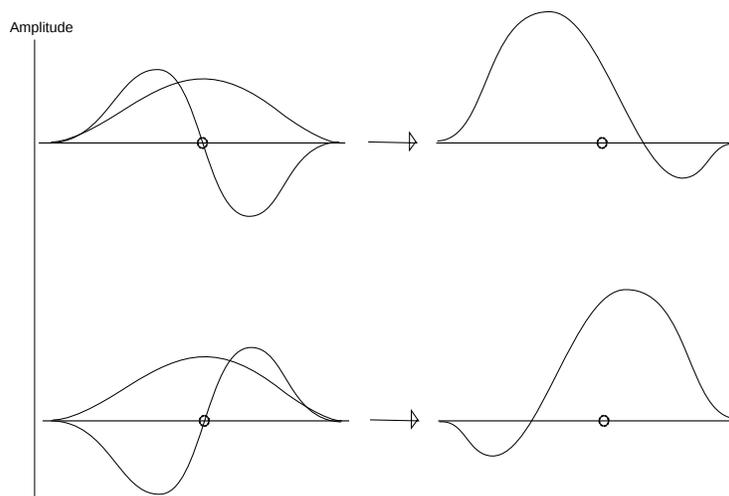
Hybrid orbitals are combinations of atomic orbitals that fit well with the 3D structures of molecules (that point in the same directions as the bonds or lone pairs). Because chemical bonding is based on Coulomb forces between electrons and nuclei, we expect that bonding electrons should spend a lot of their time between the nuclei. This is what makes a chemical bond. But what orbitals are they in when they do this? Because of the observed shapes of molecules, it seems like valence electron pairs each occupy their own area, called a domain. But the positions of these areas that we learned in the [previous section](#) don't match the positions of the [atomic orbitals](#) we studied before. We can fix this by making combinations of the atomic orbitals that have new shapes, called **hybrids**.

When are Hybrids Useful?

We mostly use hybrid orbitals to describe the bonding in organic chemistry, for compounds composed mainly of C and H. Hybrids aren't so good for molecules like SF_6 .

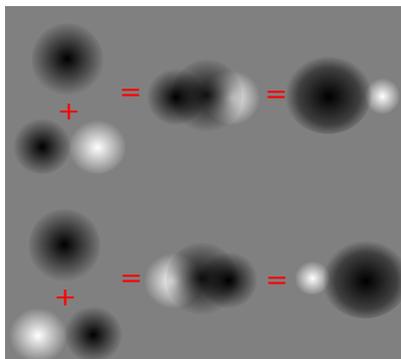
Building Hybrid Orbitals

We can build hybrid orbitals using [wave interference](#). First, let's think about a molecule like BeF_2 (in the gas phase, where it is a molecule and not an ionic solid). This molecule is [predicted to be linear](#), so how do we put the 4 bonding electrons into 2 orbitals pointed the right directions? We can imagine taking the Be 2s orbital and 2p_z orbital, and combining them in 2 ways, adding and subtracting. This gives us 2 new orbitals. (Any time you combine orbitals, you get as many out as you put in.) This is first shown using "1-D" waves, where the x-axis is radius and the y-axis is Ψ . It's important to think about the phases of the orbitals during this combination, and think about constructive and destructive interference.



The formation of sp hybrid orbitals, illustrated with approximate 1-D waves, showing Ψ vs radius. The small circle shows the position of the nucleus. We add the 2 waves on the left to get the total wave on the right.

Once you are comfortable with the wave mixing pattern in the diagram above, look at the 2-D version.

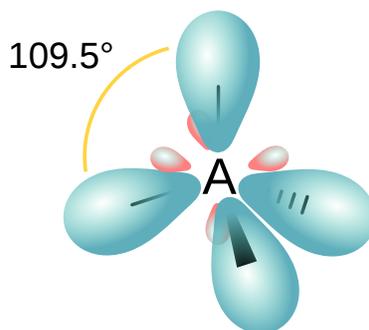


The formation of sp hybrid orbitals, illustrated with approximate 2-D drawings of atomic orbitals. Positive amplitude of Ψ is shown with black, negative amplitude of Ψ is shown with white, on a gray background. Where positive and negative amplitude waves overlap, the sum approaches zero (gray background).

You can see that by combining an s orbital and a p orbital on the same atom, we get 2 new orbitals, which point opposite directions. These orbitals are good for making 2 bonds in a linear shape, like in the molecule BeF_2 . Each of the big black lobes will make a bond with an orbital or hybrid orbital on F. In the same way, we can mix 1 s orbital and 2 p orbitals to get sp^2 hybrids, or 1 s and 3 p orbitals to get sp^3 hybrids, shown below. We use sp^2 hybrids for trigonal planar molecules like BH_3 and sp^3 orbitals for tetrahedral shapes like in CH_4 .

Important Hybrids

Although other hybrids are sometimes mentioned, the most important ones are sp , sp^2 and sp^3 . (Hybrid orbitals using d orbitals are usually not a good or useful description of what's going on.) Just remember the general shape of each of these, and what geometry molecule they match.



Important hybrid orbitals, showing the number of hybrid orbitals and the angle between them. (Left to right or top to bottom, sp , sp^2 , sp^3 .) Positive amplitude of Ψ is blue and negative amplitude of Ψ is pink. Shapes are approximate. Modified from originals by Jfmelero via Wikimedia Commons.

Outside Links

- [CrashCourse Chemistry: Orbitals](#) (10 min)
- [Khan Academy: Sp hybridization](#) (11 min)

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