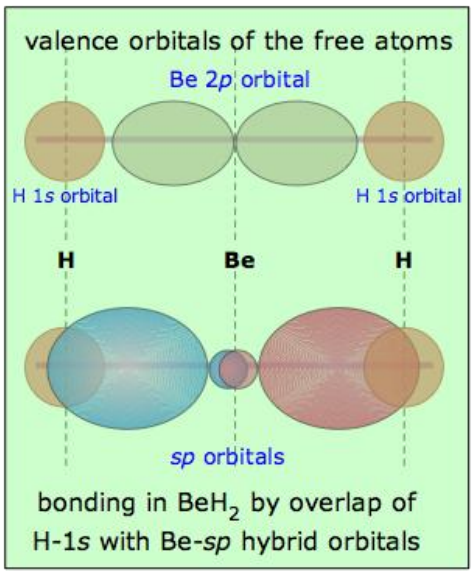
HYBRIDS DERIVED FROM ATOMIC *S*- AND *P* ORBITALS

Digonal bonding: sp-hybrid orbitals

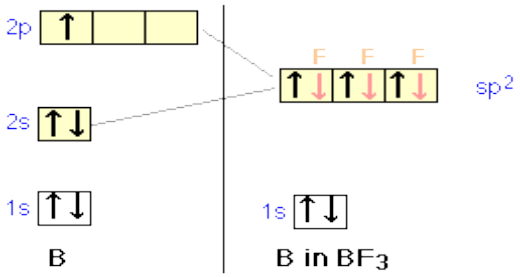
Returning to the example of BeH2, we can compare the valence orbitals in the free atoms with those in the beryllium hydride molecule as shown here. It is, of course, the overlap between the hydrogen-1sorbitals and the two lobes of the beryllium sp-hybrid orbitals that constitutes the two Be—H "bonds" in this molecule.



Notice that whereas a single p-orbital has lobes on both sides of the atom, a single sp-hybrid has most of its electron density on one side, with a minor and more spherical lobe on the other side. This minor lobe is centered on the central atom (some textbook illustrations don't get this right.)

As far as the shape of the molecule is concerned, the result is exactly the same as predicted by the VSEPR model (although hybrid orbital theory predicts the same result in a more fundamental way.)

We can expect any central atom that uses sp-hybridization in bonding to exhibit linear geometry when incorporated into a molecule.

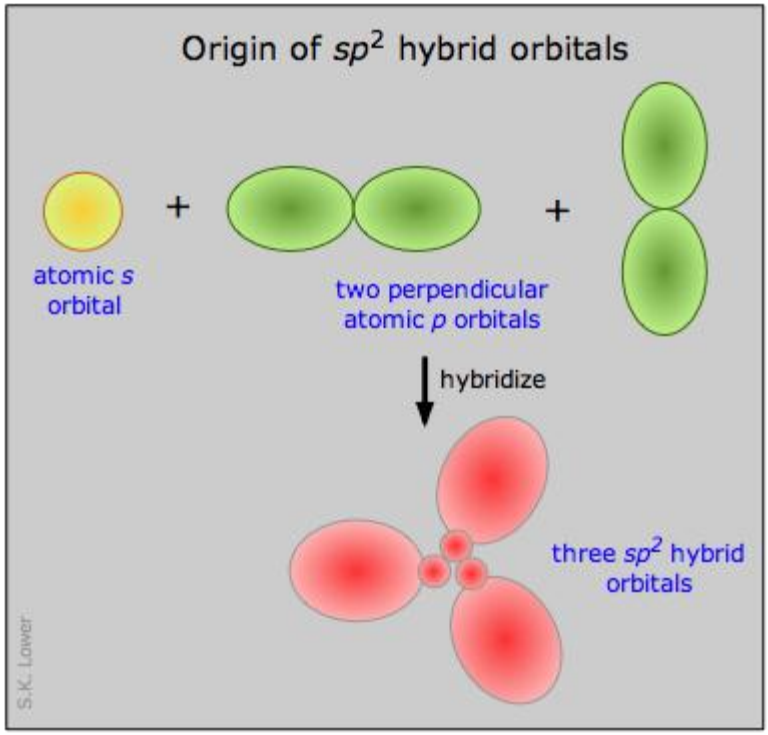


Trigonal (sp2) hybridization

We can now go on to apply the same ideas to some other simple molecules.

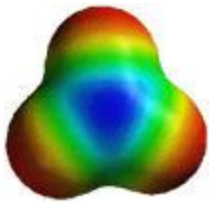
In boron trifluoride, for example, we start with the boron atom, which has three outer-shell electrons in its normal or ground state, and three fluorine atoms, each with seven outer electrons. As is shown in this configuration diagram, one of the three boron electrons is unpaired in the ground state. In order to explain the trivalent bonding of boron, we postulate that the atomic s- and p- orbitals in the outer shell of boron mix to form three equivalent hybrid orbitals. These particular orbitals are called sp2 hybrids, meaning that this set of orbitals is derived from one s- orbital and two p-orbitals of the free atom.

This illustration shows how an s-orbital mixes with two p orbitals to form a set of three sp2 hybrid orbitals. Notice again how the three atomic orbitals yield the same number of hybrid orbitals.



Boron trifluoride BF3 is a common example of sp2 hybridization.

The molecule has plane trigonal geometry.



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