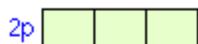
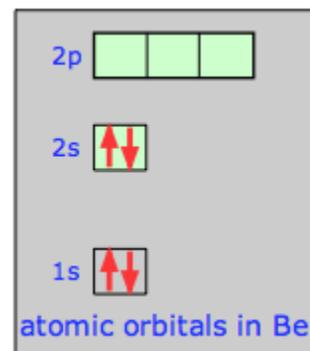


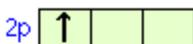
WHY ATOMIC ORBITALS DON'T WORK FOR MOLECULES

Bonding in beryllium hydride

Consider how we might explain the bonding in a compound of divalent beryllium, such as beryllium hydride, BeH_2 . The beryllium atom, with only four electrons, has a configuration of $1s^2 2s^2$. Note that the two electrons in the 2s orbital have



Be atom in ground state



Be atom in excited state

opposite spins and constitute a stable pair that has no tendency to interact with unpaired electrons on other atoms.

The only way that we can obtain two unpaired electrons for bonding in beryllium is to promote one of the 2s electrons to the 2p level. However, the energy required to produce this excited-state atom would be sufficiently great to discourage bond formation. It is observed that Be does form reasonably stable bonds with other atoms. Moreover, the two bonds in BeH_2 and similar molecules are completely equivalent; this would not be the case if the electrons in the two bonds shared be orbitals of different types, as in the "excited state" diagram above.

These facts suggest that it is incorrect to assume that the distribution of valence electrons that are shared with other atoms can be described by atomic-type s, p, and d orbitals at all.

Remember that these different orbitals arise in the first place from the interaction of the electron with the single central electrostatic force field associated with the positive nucleus. An outer-shell electron in a bonded atom will be under the influence of a force field emanating from two positive nuclei, so we would expect the orbitals in the bonded atoms to have a somewhat different character from those in free atoms. In fact, as far as valence electrons are concerned, we can throw out the concept of atomic orbital altogether and reassign the electrons to a new set of molecular orbitals that are characteristic of each molecular configuration. This approach is indeed valid, but we will defer a discussion of it until a later unit.

For now, we will look at a less-radical model that starts out with the familiar valence-shell atomic orbitals, and allows them to combine to form hybrid orbitals whose shapes conform quite well to the bonding geometry that we observe in a wide variety of molecules.

Source: <http://www.chem1.com/acad/webtext/chembond/cb06.html>