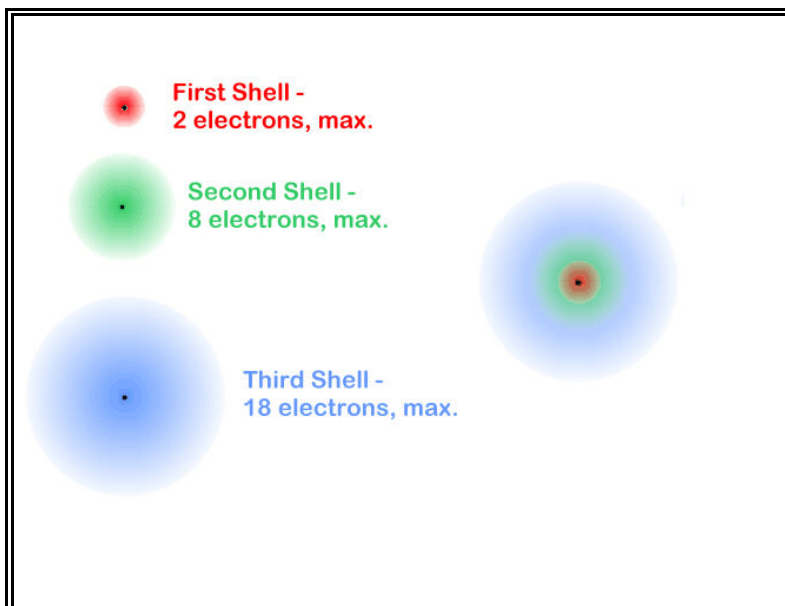


Atomic Structure – Structure of Isolated Atoms

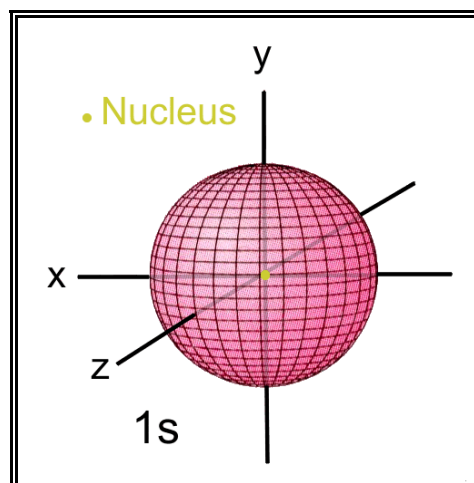
Nucleus – contains protons and neutrons.

Electrons are found in spherical “shells” around the nucleus. Shell #1 is the smallest and can accommodate up to 2 electrons. Shell #2 is larger and can accommodate up to 8 electrons. Shell #3 is larger still and can accommodate up to 18 electrons, *etc.*



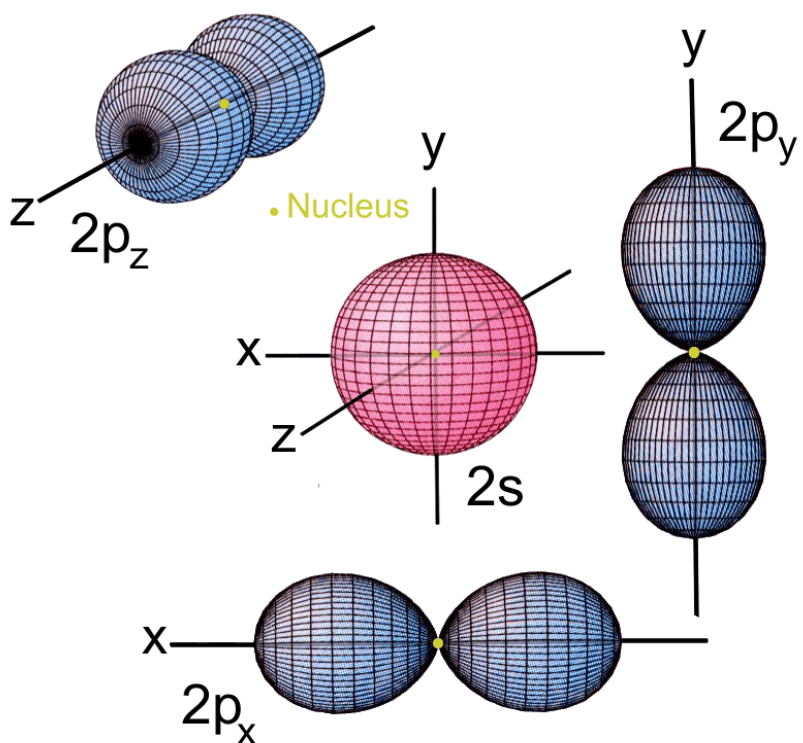
The black dot is the nucleus at the center of the atom and contains the protons and neutrons of the atom. The electrons are contained in spherical shells (shown to the left) with the nucleus at the center. The first 3 shells of an atom are shown to the right superimposed on each other; each is present at the nucleus.

Within the shells there are *atomic orbitals*. Each orbital can accommodate up to 2 electrons (Pauli principle). s-Orbitals are spheres centered at the nucleus. p-Orbitals are dumbbell shaped with the nucleus in the middle. d-Orbitals are more complex.



Shell 1: one 1s orbital.

Shell 2: one 2s orbital, three 2p orbitals – $2p_x$, $2p_y$, and $2p_z$. [Imagine that all 4 orbitals have the nucleus in common because they do. In other words, move the p orbitals so their axes overlap the corresponding axes passing through the s orbital.]



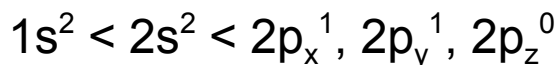
Shell 3: one 3s orbital, three 3p orbitals, five 3d orbitals.

Electrons will tend to fill orbitals in order of increasing energy:

$$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s$$

The maximum number of electrons which can be accommodated in an orbital is 2, with spins paired (Pauli principle), and when orbitals of the same energy (*degenerate* orbitals) fill, electrons fill these one at a time with the electron spins unpaired until the orbitals are all half filled (one electron each) (Hund's rule).

Consider carbon:

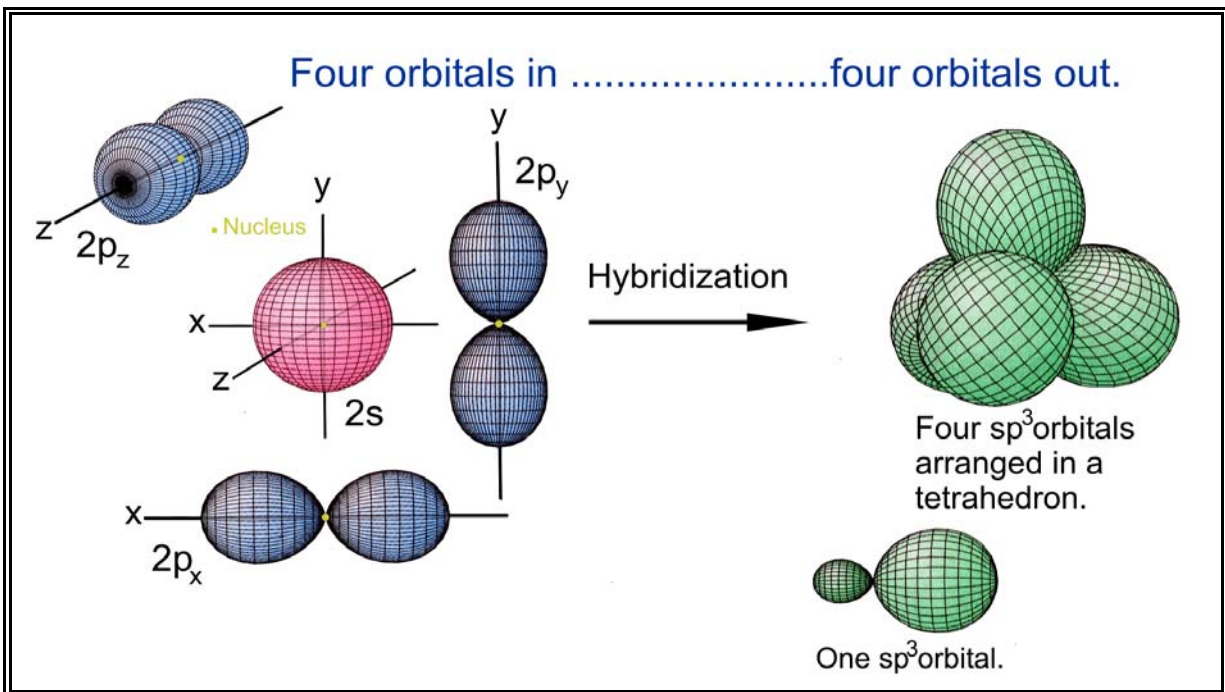


When the valence electrons (electrons in the outermost occupied shell) in an isolated carbon are used to form bonds with other atoms, they enter *molecular orbitals*, *MOs*, orbitals which extend over 2 or more atoms in a molecule. A relatively easy way for us to see how these MOs form is to transform at least some of the atomic orbitals (AOs) of the atom of interest, in our case carbon, to hybrid AOs which have the same orientation in space as the MOs they will become. [This requires some vector math *hocus pocus*, with which we shall not be concerned.] The core electrons, to a first approximation, remain in their AOs.

Let's see how this works.

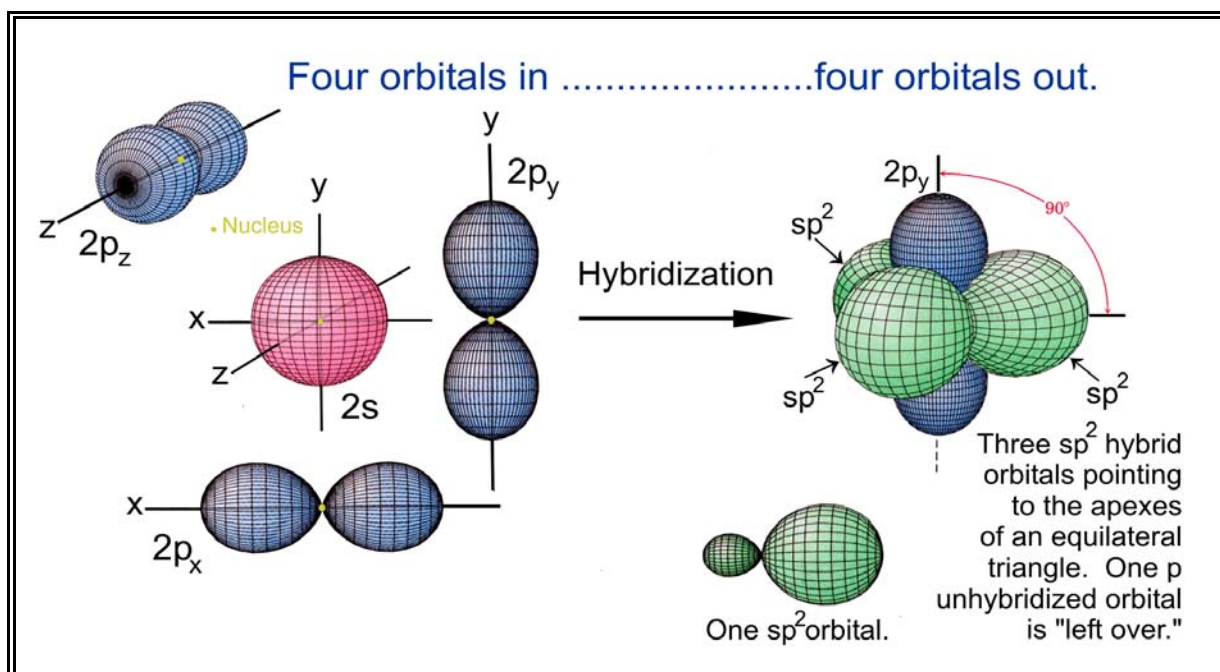
Hybrid Atomic Orbitals

1. If the atom is tetrahedral in a compound, it is sp^3 hybridized.
The 2s and the three 2p orbitals present in the uncombined atom have formed *four* sp^3 hybrid orbitals (pointing to the apexes of a tetrahedron), which may form *molecular orbitals* or may hold unshared pairs of electrons in the molecule.

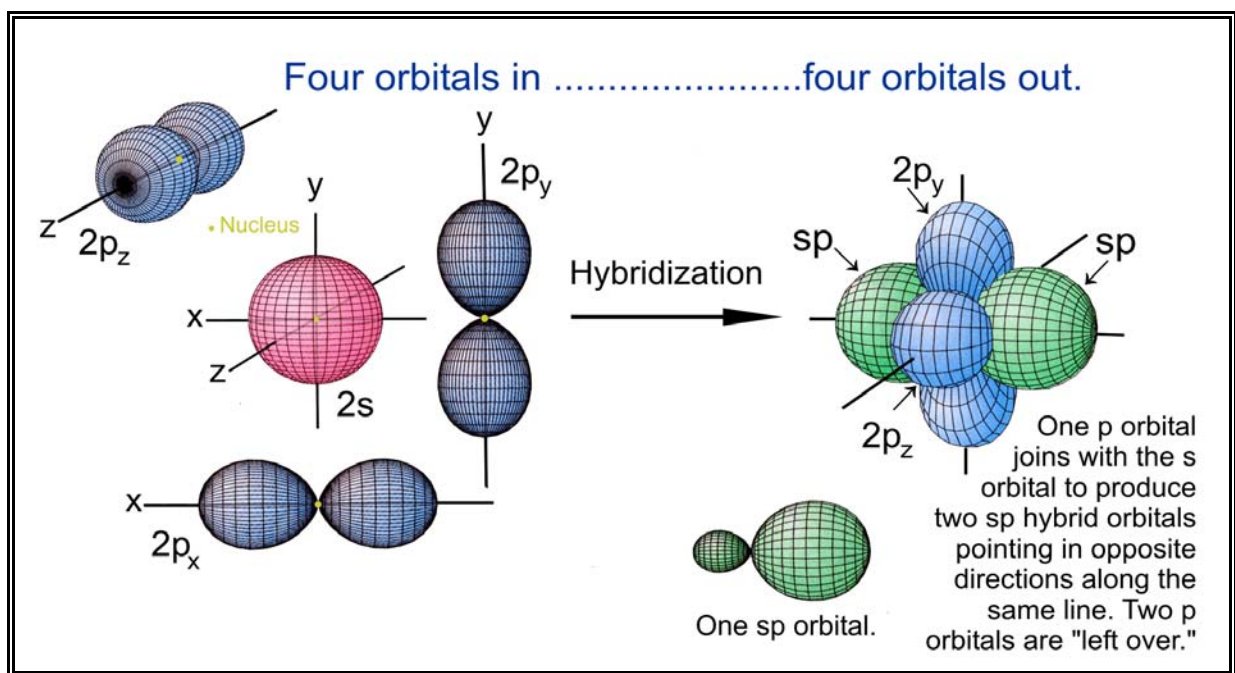


2. If the atom is trigonal in a compound, it is sp^2 hybridized.

The 2s and *two* of the three 2p orbitals present in the uncombined atom have formed *three* sp^2 hybrid orbitals (pointing to the apexes of an equilateral triangle), which may form *molecular orbitals* or may hold unshared pairs of electrons in the molecule. The 2p orbital which is not hybridized will usually form a *molecular orbital*.



3. If the atom is digonal (linear) in a compound, it is sp hybridized.
- The $2s$ and *one* of the three $2p$ orbitals present in the uncombined atom have formed *two* sp hybrid orbitals (collinear, pointing in opposite directions), which may form *molecular orbitals* or may hold unshared pairs of electrons in the molecule. The two $2p$ orbitals which are not hybridized will usually form *molecular orbitals*.



Molecular Orbitals

Orbital – Region of space around an atom or within a molecule which can accommodate one or two electrons (Pauli principle).

Orbitals associated with an atom: *atomic orbitals*.

Orbitals which result from the interaction of two or more atomic orbitals on different atoms: *molecular orbitals*.

Electrons that bond atoms together, forming molecules as a result, are found in molecular orbitals.

Types of Bonds

☞ Ionic Bonds: An atom or group of atoms donates one or more valence shell electrons to an atom or group of atoms which accepts electrons (they do this to achieve the noble gas valence shell configuration); the resulting electrostatic attraction of the charged particles (ions) for each other is known as an ionic bond.

Atoms which form ionic bonds with each other tend to differ from each other in electronegativity by more than ~ 1.7 units on the Pauling scale.

☞ Covalent Bonds: Valence shell electrons are shared between or among atoms (they do this to achieve the noble gas valence shell configuration); the positively charged atomic nuclei are mutually attracted to the negatively charged electrons in the bond and, so, held together.

Atoms which form covalent bonds with each other tend to differ from each other in electronegativity by less than ~ 1.7 units on the Pauling scale.

Atoms which are held together by covalent bonds are called molecules.