

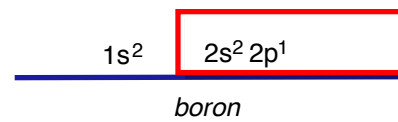
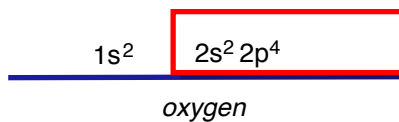
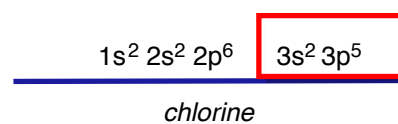
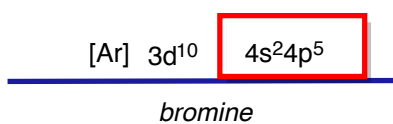
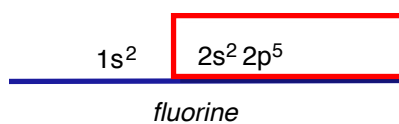
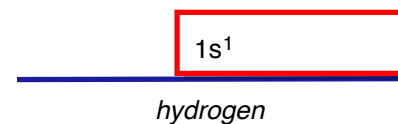
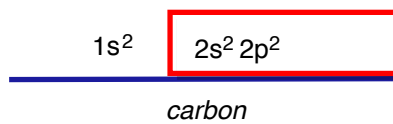
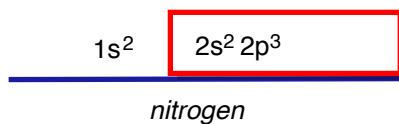
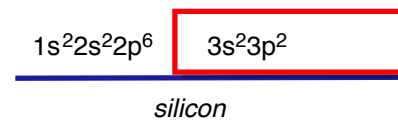
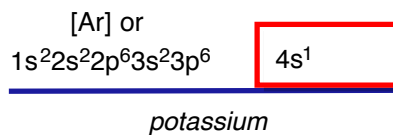
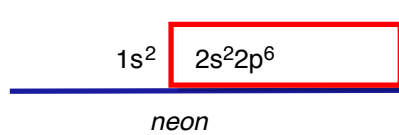
# Hybridization: The Shape Of Things To Come

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## A. Intro

## B. Electron Counting

### In Atoms



## In Molecules, and Valency

2 electrons in the first shell,  
8 in the second,  
8 in the third.

share  
completely donate or receive electrons.

each hydrogen atom has 2 first shell electrons  
One bond containing 2 electrons is formed in this sharing process  
valency of hydrogen in H<sub>2</sub> is 1

He

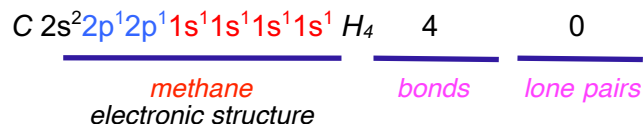
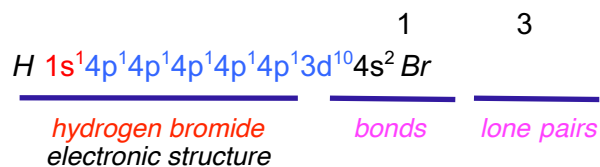
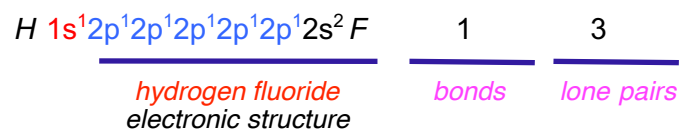
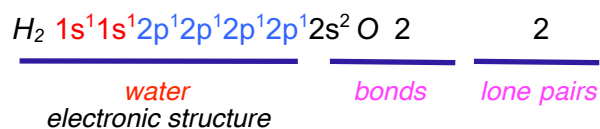
C 4 N 3 O 2 F 1 Cl 1 Br 1 S 2

may only bring 1  
common molecules is 1.

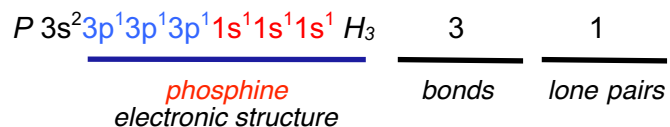
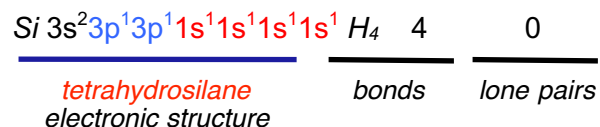
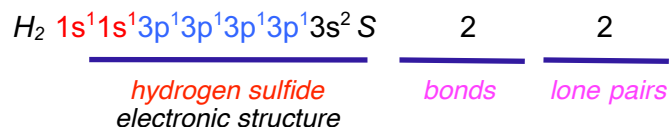
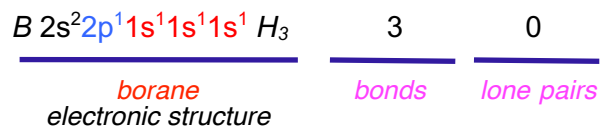
C CH<sub>4</sub> N NH<sub>3</sub> O H<sub>2</sub>O F HF Cl HCl Br HBr S H<sub>2</sub>S



The blue and red electrons are shared in bonds, two per bond, so ammonia has two electrons that are not in bonds, *ie* a lone pair.



avored electron count for that is 8



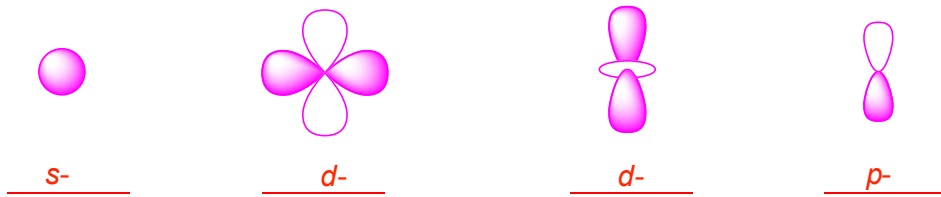
electrons is lost

## C. Mixing Atomic Orbitals To Maximize Overlap In Molecules

### Combining *s*- and *p*-Orbitals

called atomic orbitals.

have different shapes as atomic orbitals.

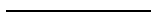


hybridized to make them.

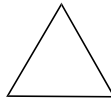
2 molecular orbitals, of three gives 3, and of  $n$  gives  $n$ .

denoted as  $sp$ , whereas  $sp^2$  surfaces are formed if two  $p$ -orbitals are mixed with one  $s$ -  
a  $sp^3$  hybrid.

### Geometric Shapes



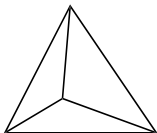
a straight line connecting three dots



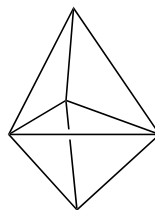
a triangle



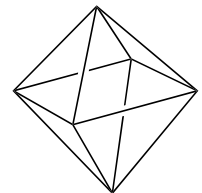
a square



a tetrahedron



a trigonal bipyramid



an octahedron

the boy in the middle.

girl-boy-girl angle is 180

ideal bond angle.

middle of a triangle with

then 120°.

a tetrahedron,

109°.

## Shapes Of Molecules Based On Geometric Shapes

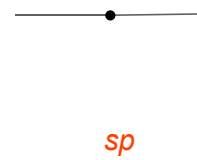
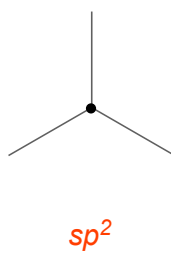
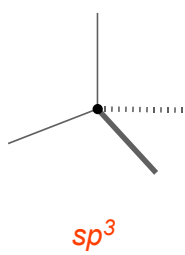
2  $sp$ -hybrid orbitals.

3 hybrid orbitals, and

4 arise from.

Bold lines mean

dashed lines



will be  $sp^2$  hybridized.

A tetrahedron of  $sp^3$  hybrids

if 4 bonds

$sp$  hybrid orbitals.

0 lone pairs

it is tetrahedral.

Fluorine in HF is surrounded by one atom, with which it shares one electron, and it has 6 electrons that it did not share, *ie* 3 lone pairs.

4 entities

hydrogen fluoride is approximately tetrahedral.

Water

4 objects

tetrahedral

hydrogen chloride, 4

Cl is tetrahedral

ammonia, 4  
tetrahedral

hydrogen sulfide, 4  
tetrahedral arrangement; and,

borane, 3  
triangular arrangement.

C in methane is tetrahedral with a dihedral angle of 109°

O in water is tetrahedral with a dihedral angle of 109°

Br in hydrogen bromide is tetrahedral with a dihedral angle of 109°

N in ammonia is tetrahedral with a dihedral angle of 109°

S in H<sub>2</sub>S is tetrahedral with a dihedral angle of 109°

B in BH<sub>3</sub> is trigonal with a dihedral angle of 120°

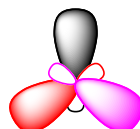
an  $sp$  hybrid consisting of 2 MOs in a linear arrangement with a dihedral angle of  $180^\circ$

3  $sp^2$  MOs, and these arrange in a trigonal arrangement with a dihedral angle of  $120^\circ$

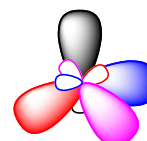
4  $sp^3$  MOs, and these arrange in a tetrahedral arrangement with a dihedral angle of  $109^\circ$



$sp$

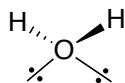


$sp^2$

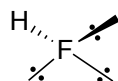


$sp^3$

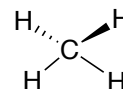
eg



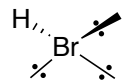
water



hydrogen fluoride



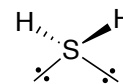
methane



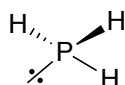
HBr



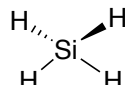
BH<sub>3</sub>



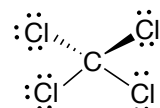
hydrogen sulfide



PH<sub>3</sub>



SiH<sub>4</sub>



CCl<sub>4</sub>

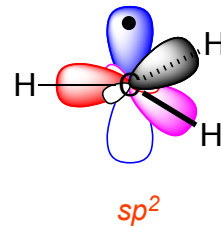
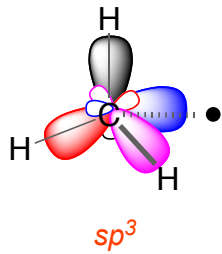


## D. Multiple Bonds

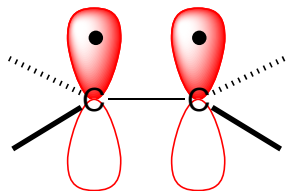
8 electrons in its second shell

7 electrons in its second shell; this *is not* a *are* relatively reactive.

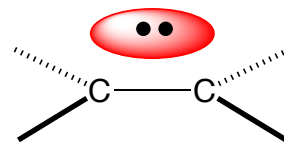
$sp^3$  hybridized



$\sigma$ -bonded sp hybridized C-atoms



ethene *before* mixing  
p-orbitals



ethene *after* mixing  
p-orbitals

are called sigma.

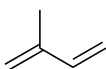
pi bond.

Maximal overlap is achieved

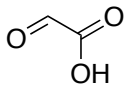
Perpendicular p-orbitals do not interact.

of a pi bond.

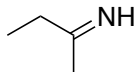
1 line(s), and  $\pi$ -bonds are represented by adding 2 parallel line(s).



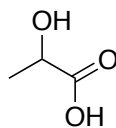
# 2  
isoprene



# 2  
pyruvic acid



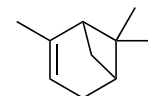
# 1  
an imine



# 1  
lactic acid



# 3  
benzene



# 1  
 $\beta$ -pinene

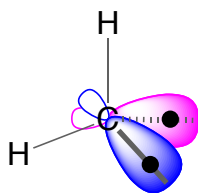
because they would not contribute to the binding interaction.

Atoms in molecules can selectively

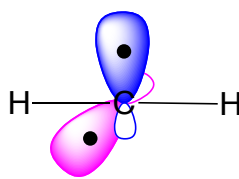
Carbene, CH<sub>2</sub>, 6 shared electrons in the C-second shell.

this is called the singlet state.

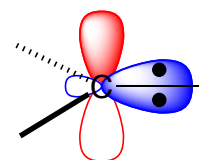
Alternatively, carbenes can be  $sp^2$ -hybridized with one electron in each of the hybrid lobes that does not point to a hydrogen; this is a triplet state.



*triplet*

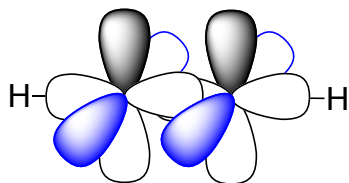


*unstable triplet*

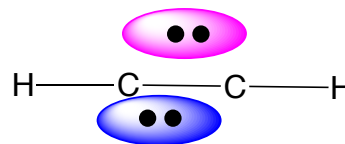


*singlet*

$\sigma$ -bonded sp hybridized C-atoms



*ethyne before mixing  
p-orbitals*

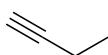


*ethyne after mixing  
p-orbitals*

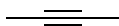
two  $\pi$  bonds surrounding the  $\sigma$  bond called a triple bond.



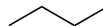
# 1  
propyne



# 1  
1-butyne



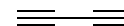
# 1  
2-butyne



# 0  
butane



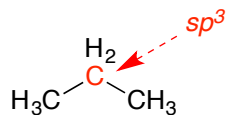
# 1  
acetonitrile



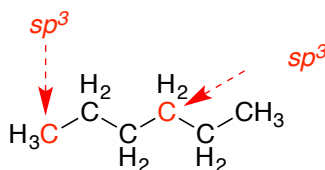
# 2  
1,3-butadiene

it does not matter if.

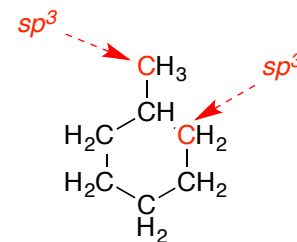
are sp hybridized, three sp<sup>2</sup>, and four sp<sup>3</sup>.



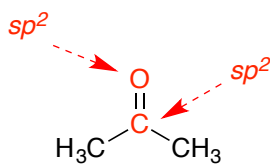
propane



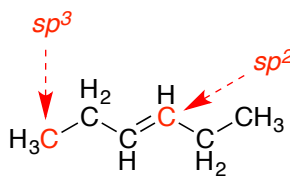
hexane



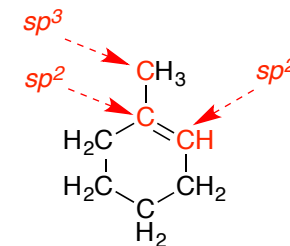
methylcyclohexane



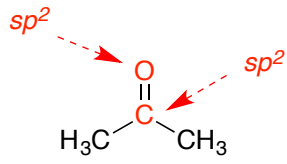
acetone



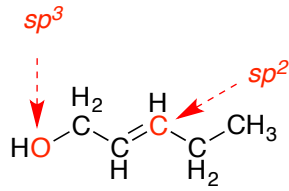
1-pentene



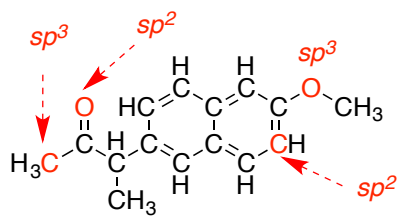
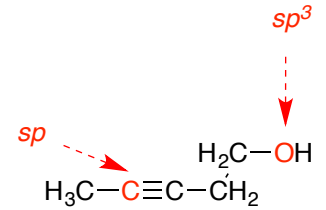
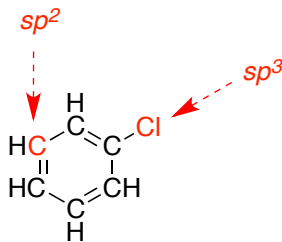
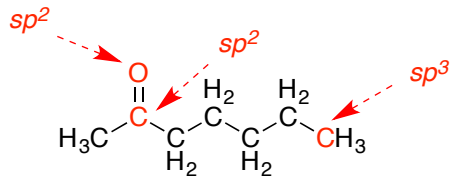
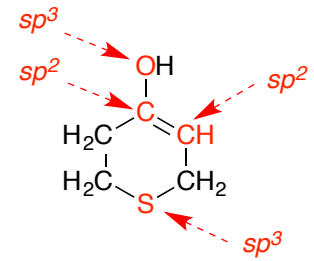
1-methylcyclohexene



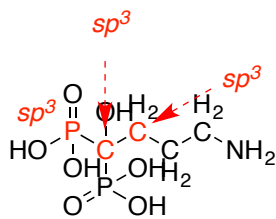
acetic acid



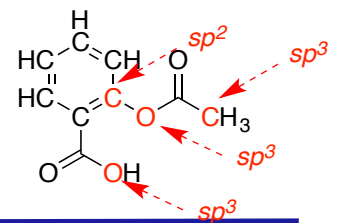
cis-1-hydroxy-2-butene



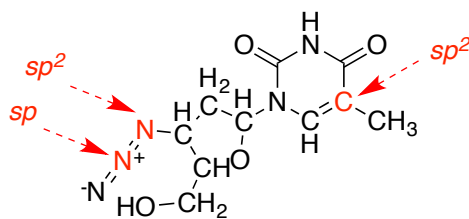
naproxen



alendronate



aspirin



zidovudine (AZT)