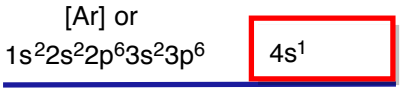
Hybridization: The Shape Of Things To Come

A. Intro

B. Electron Counting

In Atoms

neon



potassium

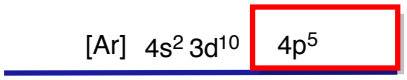
silicon

nitrogen

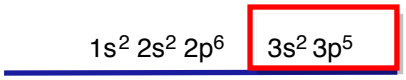
carbon

hydrogen

fluorine

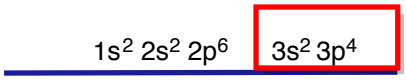


bromine



chlorine

oxygen



sulfur

boron

In Molecules, and Valency

2 electrons in the first shell,
8 in the second,
16 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_2 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_4__ *N* __NH_3___ *O* __H_2O___ *F* __HF____ *Cl* ___HCl___ *Br* __HBr____ *S* __H_2S___

N $2s^2 2p^1 2p^1 2p^1 1s^1 1s^1 1s^1$ H_3

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.

H_2 $1s^1 1s^1 2p^1 2p^1 2p^1 2p^1 2s^2$ *O*	2	2	
water electronic structure	*bonds*	*lone pairs*	

H $1s^1 2p^1 2p^1 2p^1 2p^1 2p^1 2s^2$ *F*	1	3	
hydrogen fluoride electronic structure	*bonds*	*lone pairs*	

H $1s^1 4p^1 4p^1 4p^1 4p^1 4p^1 3d^{10} 4s^2$ *Br*	1	3	
hydrogen bromide electronic structure	*bonds*	*lone pairs*	

C $2s^2 2p^1 2p^1 1s^1 1s^1 1s^1 1s^1$ H_4	4	0	
methane electronic structure	*bonds*	*lone pairs*	

favored electron count for that is *8*

B $2s^2 2p^1 1s^1 1s^1 1s^1$ H_3	3	0	
borane electronic structure	*bonds*	*lone pairs*	

H_2 $1s^1 1s^1 3p^1 3p^1 3p^1 3p^1 3s^2$ *S*	2	2	
hydrogen sulfide electronic structure	*bonds*	*lone pairs*	

Si $3s^2 3p^1 3p^1 1s^1 1s^1 1s^1 1s^1$ H_4	4	0	
tetrahydrosilane electronic structure	*bonds*	*lone pairs*	

P $3s^2 3p^1 3p^1 3p^1 1s^1 1s^1 1s^1$ H_3	3	1	
phosphine electronic structure	*bonds*	*lone pairs*	

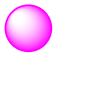
electrons *is* lost

C. Mixing Atomic Orbitals To Maximize Overlap In Molecules

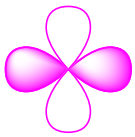
Combining *s*- and *p*-Orbitals

called *atomic* orbitals.

have *different* shapes as atomic orbitals.



s-



d-

d-

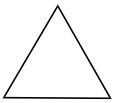
p-

hybridized to make them.
2 molecular orbitals, of three gives *3*, and of *n* gives *n*.

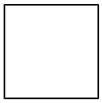
denoted as *sp*, whereas sp^2 surfaces are formed if *two p*-orbitals are mixed with one *s*-.
a ___sp^3___ hybrid.

Geometric Shapes

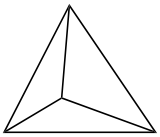
straight line connecting three dots



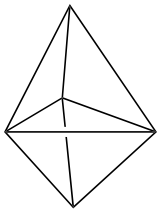
a triangle



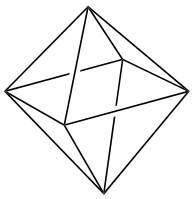
a square



a tetrahedron



a trigonal bipyramid



an octahedron

the boy *in the middle*.
girl-boy-girl angle is *180*
ideal bond angle.

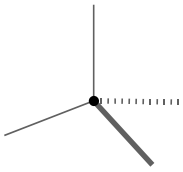
middle of a *triangle* with
then *120°*.

a *tetrahedron*,
109°.

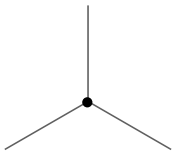
Shapes Of Molecules Based On Geometric Shapes

2 *sp*-hybrid orbitals.
3 hybrid orbitals, and
4 arise from.

Bold lines mean
dashed lines



sp^3



sp^2

sp

will be sp^2 hybridized.
A tetrahedron of sp^3 hybrids
if 4 bonds
sp hybrid orbitals.

0 lone pairs
it is *tetrahedral*.

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_2S is *tetrahedral* with a dihedral angle of *109°*

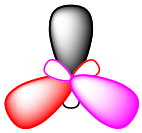
B in BH_3 is *trigonal* with a dihedral angle of *120°*

an *sp* hybrid consisting of *2* MOs in a *linear* arrangement with a dihedral angle of *180°*

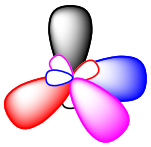
3 sp^2 MOs, and these arrange in a *trigonal* arrangement with a dihedral angle of *120°*

4 sp^3 MOs, and these arrange in a *tetrahedral* arrangement with a dihedral angle of *109°*

sp

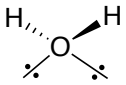


sp^2

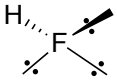


sp^3

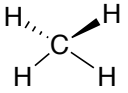
eg



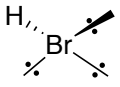
water



hydrogen fluoride

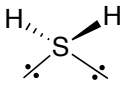


methane

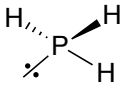


HBr

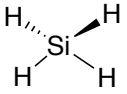
BH_3



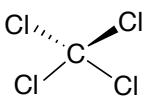
hydrogen sulfide



PH_3



SiH_4



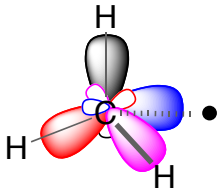
CCl_4

D. Multiple Bonds

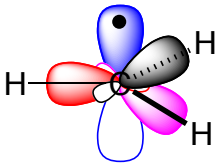
8 electrons in its second shell

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

sp^3 hybridized

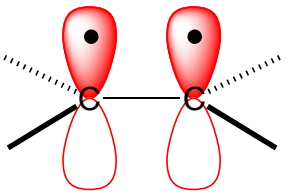


sp^3

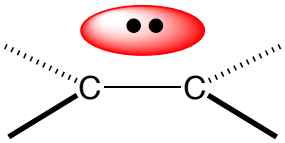


sp^2

σ-bonded *sp* hybridized *C*-atoms



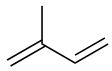
*ethene **before** mixing p-orbitals*



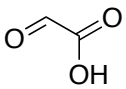
*ethene **after** mixing p-orbitals*

are called *sigma*.
pi bond.
Maximal overlap *is* achieved
Perpendicular *p*-orbitals *do* interact.

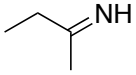
of a *π* bond.
1 line(s), and π-bonds are represented by adding *2* parallel line(s).



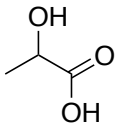
 # __2__
isoprene



 # __2__
pyruvic acid

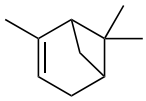


 # __1__
an imine



 # __1__
lactic acid

 # _3___
benzene



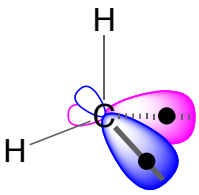
 # __1__
β-pinene

because they *would not* contribute to the binding interaction.
Atoms in molecules *can* selectively

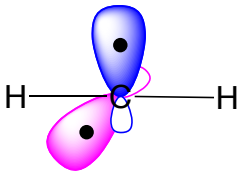
Carbene, CH_2, 6 shared electrons in the *C*-second shell.

this is called the *singlet* state.

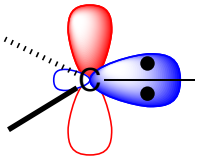
Alternatively, carbenes can be sp^2-hybridized with one electron in each of the hybrid lobes that does not point to a hydrogen; this is a *triplet* state.



triplet

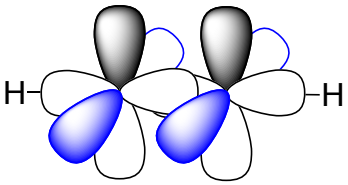


unstable triplet

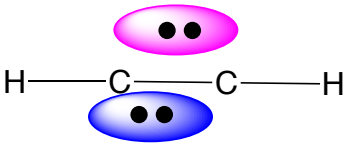


singlet

σ-bonded *sp* hybridized *C*-atoms



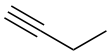
*ethyne **before** mixing p-orbitals*



*ethyne **after** mixing p-orbitals*

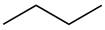
two π bonds surrounding the σ bond
called a *triple* bond.

__1__
propyne



__1__
1-butyne

__1__
2-butyne



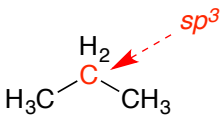
__0__
butane

__1__
acetonitrile

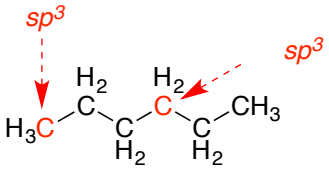
__2__
1,3-butadiyne

it *does not* matter if.

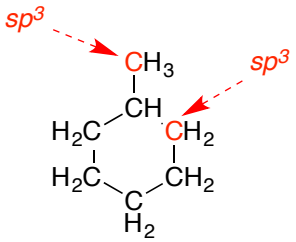
are *sp* hybridized, three *sp*^{2}, and four *sp*^{3}.



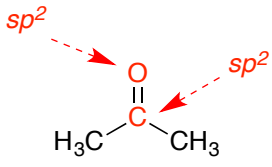
propane



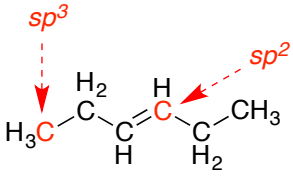
hexane



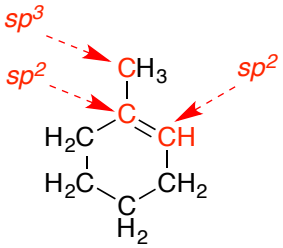
methylcyclohexane



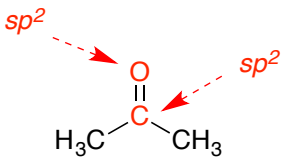
acetone



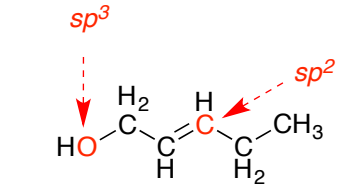
1-pentene



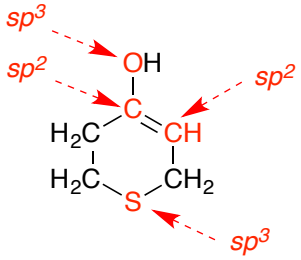
1-methylcyclohexene

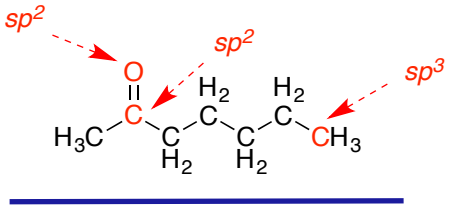


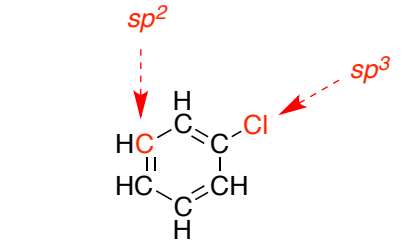
acetic acid

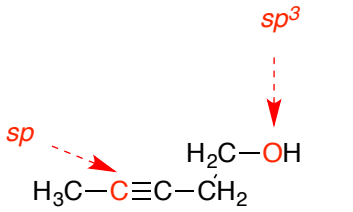


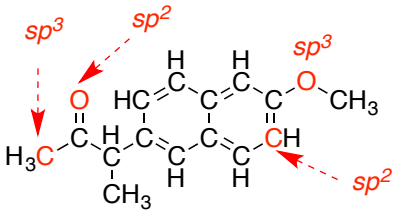
cis-1-hydroxy-2-butene



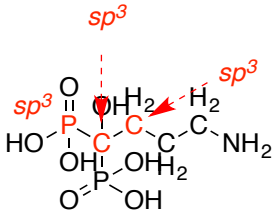




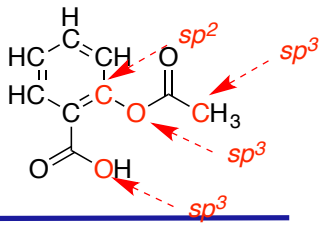




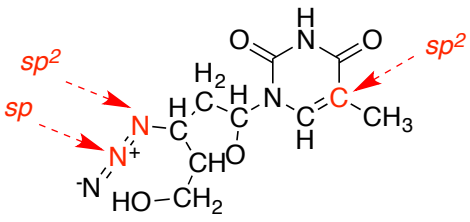
naproxen



alendronate



aspirin



zidovudine (AZT)