Hybridization: The Shape Of Things To Come

A. Intro

B. Electron Counting

In Atoms

$1s^2$ [$2s^2 2p^6$] *neon*	[Ar] or $1s^2 2s^2 2p^6 3s^2 3p^6$ [$4s^1$] *potassium*	$1s^2 2s^2 2p^6$ [$3s^2 3p^2$] *silicon*
$1s^2$ [$2s^2\,2p^3$] *nitrogen*	$1s^2$ [$2s^2\,2p^2$] *carbon*	[$1s^1$] *hydrogen*
$1s^2$ [$2s^2\,2p^5$] *fluorine*	[Ar] $3d^{10}$ [$4s^2 4p^5$] *bromine*	$1s^2\ 2s^2\ 2p^6$ [$3s^2\ 3p^5$] *chlorine*
$1s^2$ [$2s^2\,2p^4$] *oxygen*	$1s^2\ 2s^2\ 2p^6$ [$3s^2\ 3p^4$] *sulfur*	$1s^2$ [$2s^2\,2p^1$] *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 $2s^2 2p^1 2p^1 2p^1 1s^1 1s^1 1s^1$ *H₃*

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

1 3

H $1s^1 4p^1 4p^1 4p^1 4p^1 4p^1 3d^{10} 4s^2$ Br

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

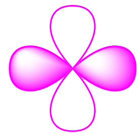
C. Mixing Atomic Orbitals To Maximize Overlap In Molecules

Combining *s*- and *p*-Orbitals

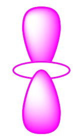
called *atomic* orbitals.

have *different* shapes as atomic orbitals.

s-



d-



d-

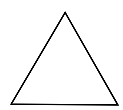
p-

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

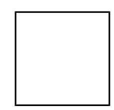
denoted as *sp*, whereas sp^2 surfaces are formed if *two p*-orbitals are mixed with one *s*-.
a ____sp^3___ hybrid.

Geometric Shapes

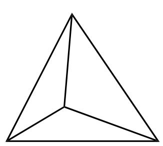
straight line connecting three dots



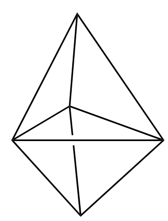
a triangle



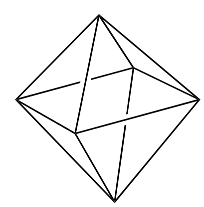
a square



a tetrahedron



a trigonal bipyramid



an octahedron

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

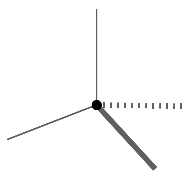
middle of a *triangle* with
then *120°*.

a *tetrahedron*,
109°.

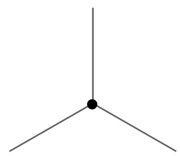
Shapes Of Molecules Based On Geometric Shapes

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°*

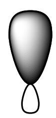
S in H_2S is *tetrahedral* with a dihedral angle of *109°*

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

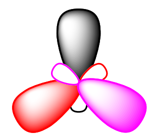
an *sp* hybrid consisting of *2* MOs in a *linear* arrangement with a dihedral angle of *180°*

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

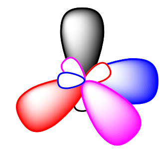
4 sp^3 MOs, and these arrange in a *tetrahedral* arrangement with a dihedral angle of *109°*



sp

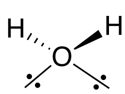


sp^2

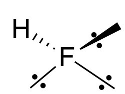


sp^3

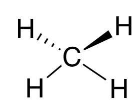
eg



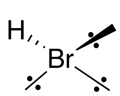
water



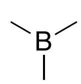
hydrogen fluoride



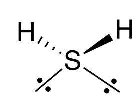
methane



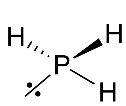
HBr



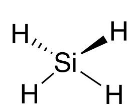
BH_3



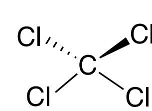
hydrogen sulfide



PH_3



SiH_4



CCl_4

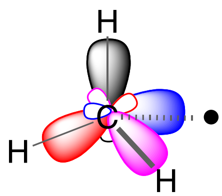
D. Multiple Bonds

8 electrons in its second shell

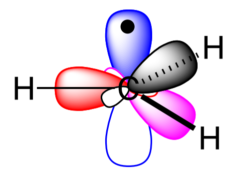
7 electrons in its second shell; this *is not* a

are relatively reactive.

sp^3 hybridized

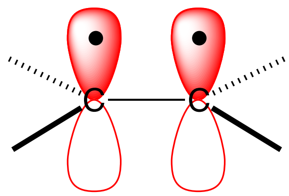


sp^3

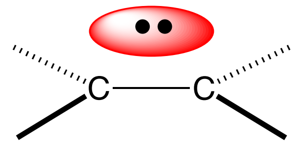


sp^2

σ-bonded *sp* hybridized *C*-atoms



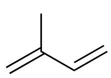
*ethene **before** mixing*
p-orbitals



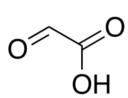
*ethene **after** mixing*
p-orbitals

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

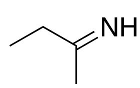
of a π bond.
1 line(s), and π-bonds are represented by adding *2* parallel line(s).



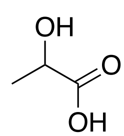
__2__
isoprene



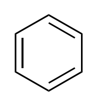
__2__
pyruvic acid



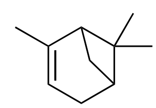
__1__
an imine



__1__
lactic acid



_3___
benzene



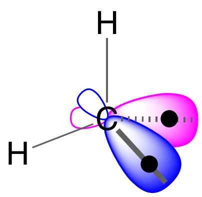
__1__
β-pinene

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

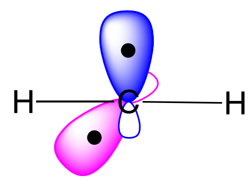
Carbene, CH_2, *6* shared electrons in the *C*-second shell.

this is called the *singlet* state.

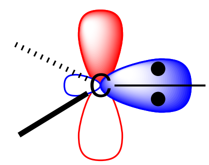
Alternatively, carbenes can be sp^2-hybridized with one electron in each of the hybrid lobes that does not point to a hydrogen; this is a *triplet* state.



triplet

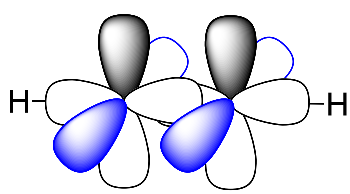


unstable triplet

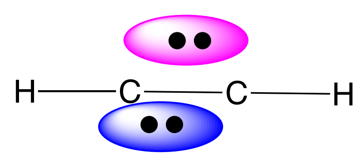


singlet

σ-bonded *sp* hybridized *C*-atoms

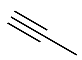


ethyne ***before*** *mixing p-orbitals*

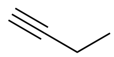


ethyne ***after*** *mixing p-orbitals*

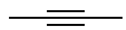
two π bonds surrounding the σ bond
called a *triple* bond.



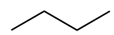
__1__
propyne



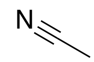
__1__
1-butyne



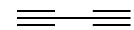
__1__
2-butyne



__0__
butane



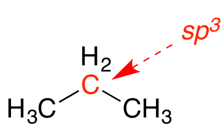
__1__
acetonitrile



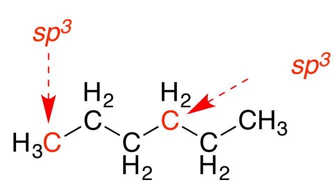
__2__
1,3-butadiyne

it *does not* matter if.

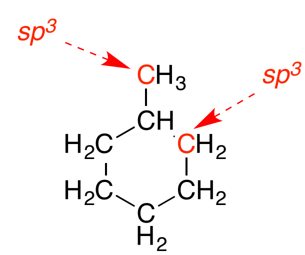
are *sp* hybridized, three *sp^2*, and four *sp^3*.



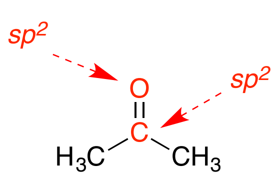
propane



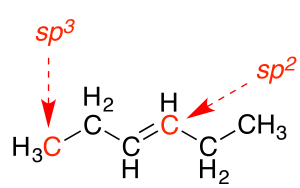
hexane



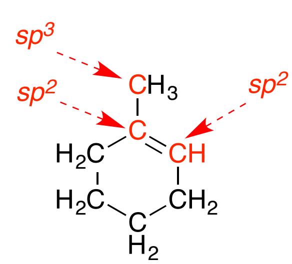
methylcyclohexane



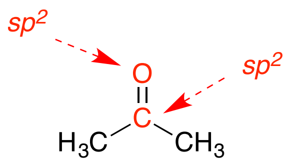
acetone



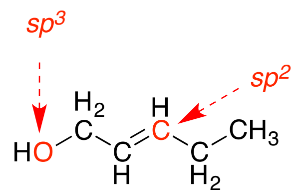
1-pentene



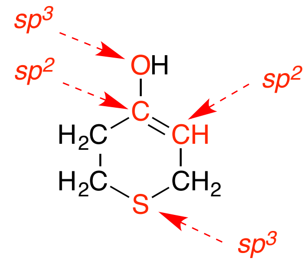
1-methylcyclohexene

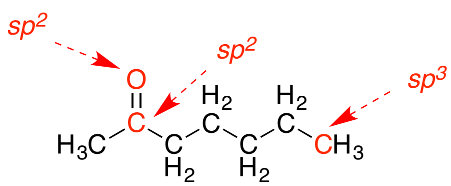


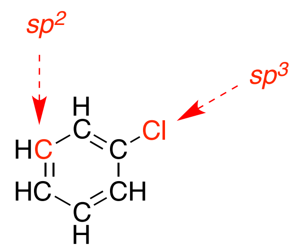
acetic acid

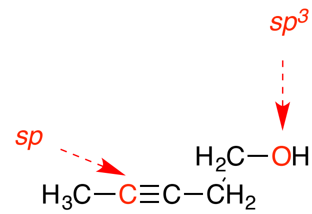


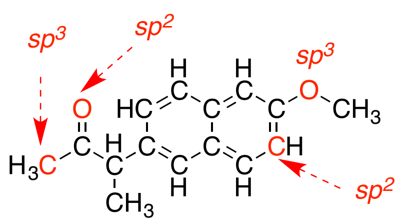
cis-1-hydroxy-2-butene



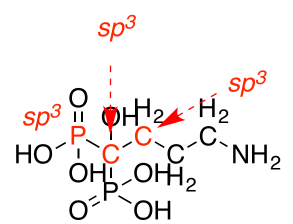




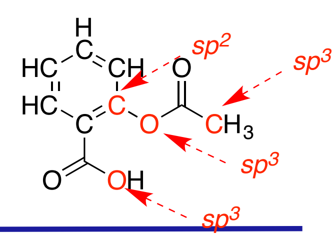




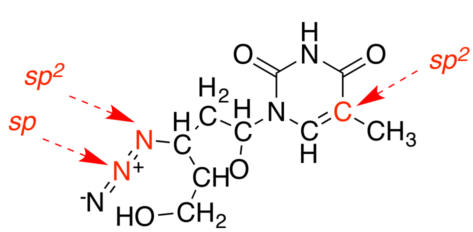
naproxen



alendronate



aspirin



zidovudine (AZT)