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,
8 in the third.

are formed when atoms *share* to form stable
ionic bonds are formed when atoms *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*

The electronic structure of *He*

C ___4_____ *N* ___3_____ *O* _____2___ *F* ___1_____ *Cl* ___1_____ *Br* ___1_____ *S* ___2_____

hydrogen atom may only bring *1* electron(s)
hydrogen in common molecules is *1*.

C ___CH_4___ *N* ___NH_3____ *O* ___H_2O___ *F* ___HF_____ *Cl* ___HCl___ *Br* ___HBr_____ S ___H_2S___

electronic structure	bonds	lone pairs
H_2 $1s^1 1s^1 2p^1 2p^1 2p^1 2p^1 2s^2$ O — *water*	2	2
H $1s^1 2p^1 2p^1 2p^1 2p^1 2p^1 2s^2$ F — *hydrogen fluoride*	1	3
H $1s^1 4p^1 4p^1 4p^1 4p^1 4p^1 3d^{10} 4s^2$ Br — *hydrogen bromide*	1	3
C $2s^2 2p^1 2p^1 1s^1 1s^1 1s^1 1s^1$ H_4 — *methane*	4	0
B $2s^2 2p^1 1s^1 1s^1 1s^1$ H_3 — *borane*	3	0
H_2 $1s^1 1s^1 3p^1 3p^1 3p^1 3p^1 3s^2$ S — *hydrogen sulfide*	2	2
Si $3s^2 3p^1 3p^1 1s^1 1s^1 1s^1 1s^1$ H_4 — *tetrahydrosilane*	4	0
P $3s^2 3p^1 3p^1 3p^1 1s^1 1s^1 1s^1$ H_3 — *phosphine*	3	1

atomic origin of electrons *is* lost

C. Mixing Atomic Orbitals To Maximize Overlap In Molecules

Combining *s*- and *p*-Orbitals

refer to where some electrons *have maximum probability of being*.

have *different* shapes as atomic orbitals.

s- *d-* *d-* *p-*

atomic orbitals that are mixed or *hybridized* to make them.

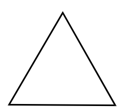
2 molecular orbitals, of three gives *3*, and of *n* gives *n*.

one *s*- and one *p*-orbital gives a *sp*-hybrid, whereas *sp^2*-orbitals are formed if *two* *p*-orbitals are mixed with one *s*-.

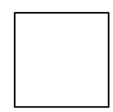
three *p*- and one *s*-orbitals gives a ___*sp^3*__-hybrid.

Geometric Shapes

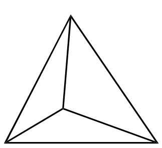
straight line connecting three dots



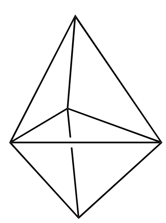
a triangle



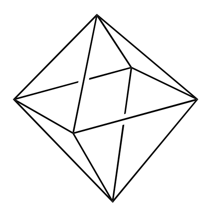
a square



a tetrahedron



a trigonal bipyramid



an octahedron

a line with the boy *in the middle.*

girl-boy-girl angle is *180°*
this is called the *ideal bond* angle.

herself in the middle of a *triangle* with
then *120°*.

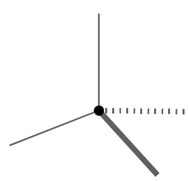
with the point in the middle of a *tetrahedron*,
then the bond angle is *109°*.

Shapes Of Molecules Based On Geometric Shapes

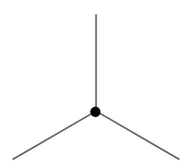
one *s*- and one *p*- atomic orbitals gives *2* *sp*-hybrid orbitals.

one *s*- and two *p*-orbitals give *3* hybrid orbitals
and *4* arise from one *s*- and three *p*-orbitals

Bold lines mean “emerges from the plane of the paper” and *dashed* lines indicate “projects behind the plane”.



sp^3



sp^2

sp

central atom will be sp^2-hybridized.

A tetrahedron of sp^3-hybrids will be formed if *4* bonds and/or lone pairs
is generated from two *sp*-hybrid orbitals.

it has *0* lone pairs
therefore it is *tetrahedral*.

and it has *6* electrons that it did not share, *ie* *3* lone pairs.

that fluoride has *4* entities

hydrogen fluoride is approximately *tetrahedral*.

Water, *oxygen* is surrounded by *4* objects
O-geometry is *tetrahedral*

hydrogen chloride, *chlorine* is surrounded by *4* objects
Cl-geometry is *tetrahedral*

ammonia, *nitrogen* is surrounded by *4* objects
N-geometry is *tetrahedral*

hydrogen sulfide, *sulfur* is surrounded by 4 objects
S-atom is at the center of a *tetrahedral* arrangement

borane, *boron* is surrounded by *3* objects
B-atom is at the center of a *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°*

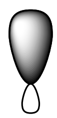
S in H_2S is *tetrahedral* with a dihedral angle of *109°*

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

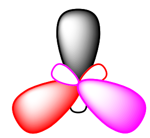
sp-hybrid consisting of *2* MOs in a *linear* arrangement with a dihedral angle of *180°*

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

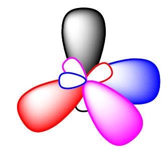
4 sp^3 MOs, and these arrange in a *tetrahedral* arrangement with a dihedral angle of *109°*



sp

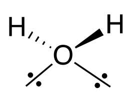


sp^2

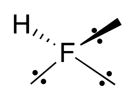


sp^3

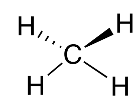
eg



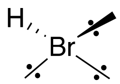
water



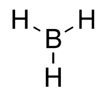
hydrogen fluoride



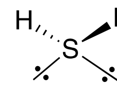
methane



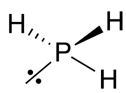
HBr



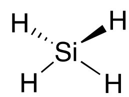
BH_3



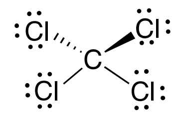
hydrogen sulfide



PH_3



SiH_4

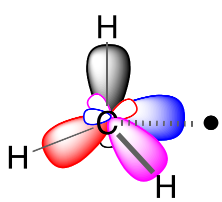


CCl_4

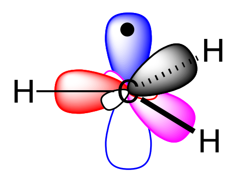
D. Multiple Bonds

the *C*-atom after sharing has *8* electrons in its second shell
the *C*-atom shares *7* electrons in its second shell; this *is not* a particularly favorable
why methyl radicals *are* relatively reactive.

Methyl radicals could be *sp^3*-hybridized



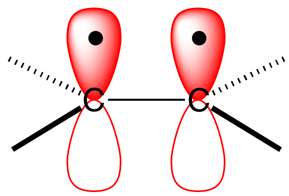
sp^3



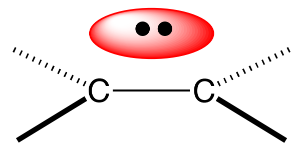
sp^2

σ-bonds are formed between two orbitals that *point directly at each other.*
π-bonds are formed between two orbitals that *are parallel.*

σ-bonded *sp*^{2}-hybridized *C*-atoms



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



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

new MO in ethene contains *2* electrons.

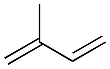
combining *sp*^{n}-hybrids (*n* = 1 – 3) at each other are σ.

p-orbitals mix they form a π-orbital.

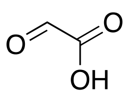
p-orbitals when they are *aligned*.
Perpendicular *p*-orbitals *do not* interact because the signs of the wave equations *cancel* in regions

sp^2-hybridization is stabilized by formation of a π-bond.

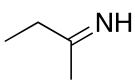
σ-bonds are represented by *1* line(s),
both one σ- and one π-bond are represented by *2* parallel line(s), so they are called *double bonds*.



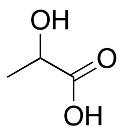
__2__
isoprene



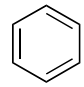
__2__
pyruvic acid



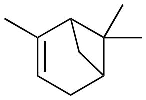
__1__
an imine



__1__
lactic acid



_3___
benzene



__1__
β-pinene

Electrons in hybridized atoms *can* occupy hybrid orbitals

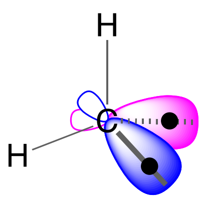
Atoms in molecules *can* selectively

highly reactive species because it has only *6* electrons

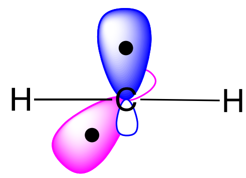
this is called the *singlet* state.

this is a *triplet* state.

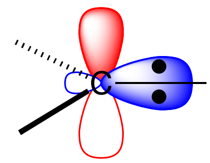
Another possibility is a *sp*-hybridized



triplet

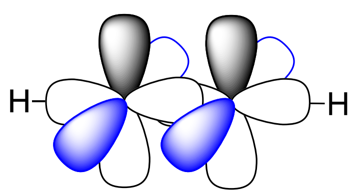


unstable triplet

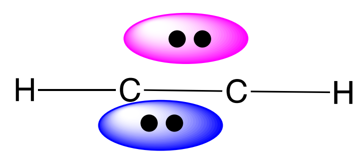


singlet

σ-bonded *sp*-hybridized *C*-atoms

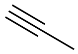


*ethyne **before** mixing*
p-orbitals

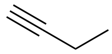


*ethyne **after** mixing*
p-orbitals

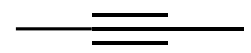
two π bonds surrounding the σ bond
called a *triple* bond.



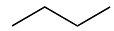
__1__
propyne



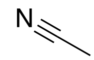
__1__
1-butyne



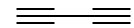
__1__
2-butyne



__0__
butane



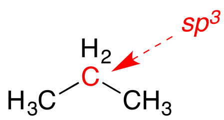
__1__
acetonitrile



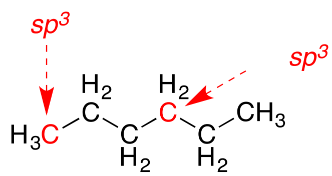
__2__
1,3-butadiyne

it *does not* matter if multiple or single

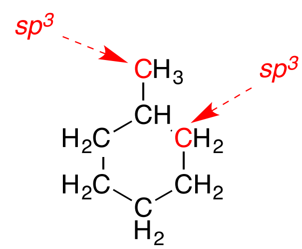
are *sp*-hybridized, three sp^2, and four sp^3.



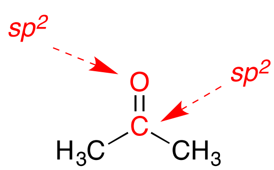
propane



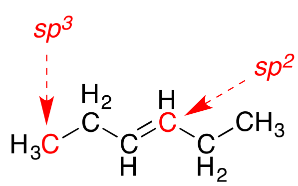
hexane



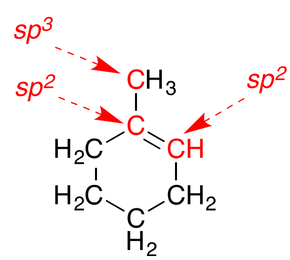
methylcyclohexane



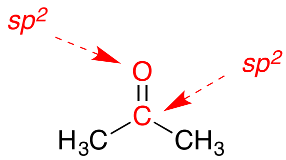
acetone



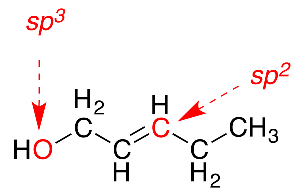
1-pentene



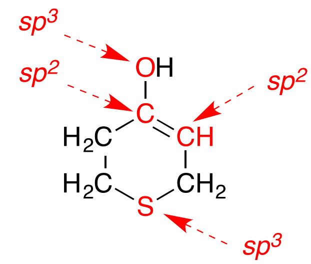
1-methylcyclohexene

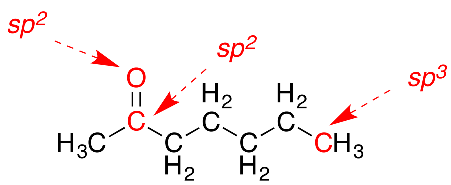


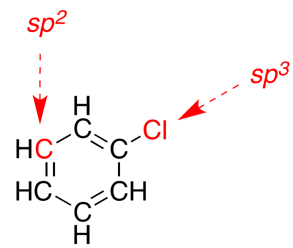
acetic acid

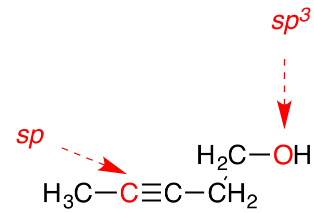


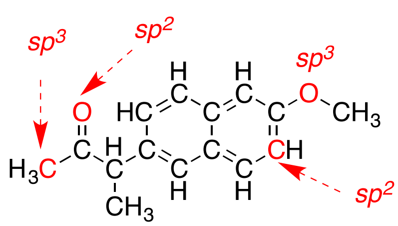
cis-1-hydroxy-2-butene



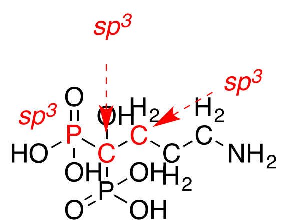




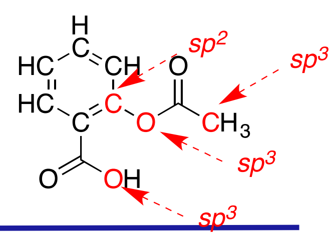




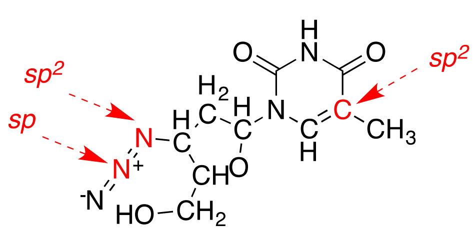
naproxen



alendronate



aspirin



zidovudine (AZT)