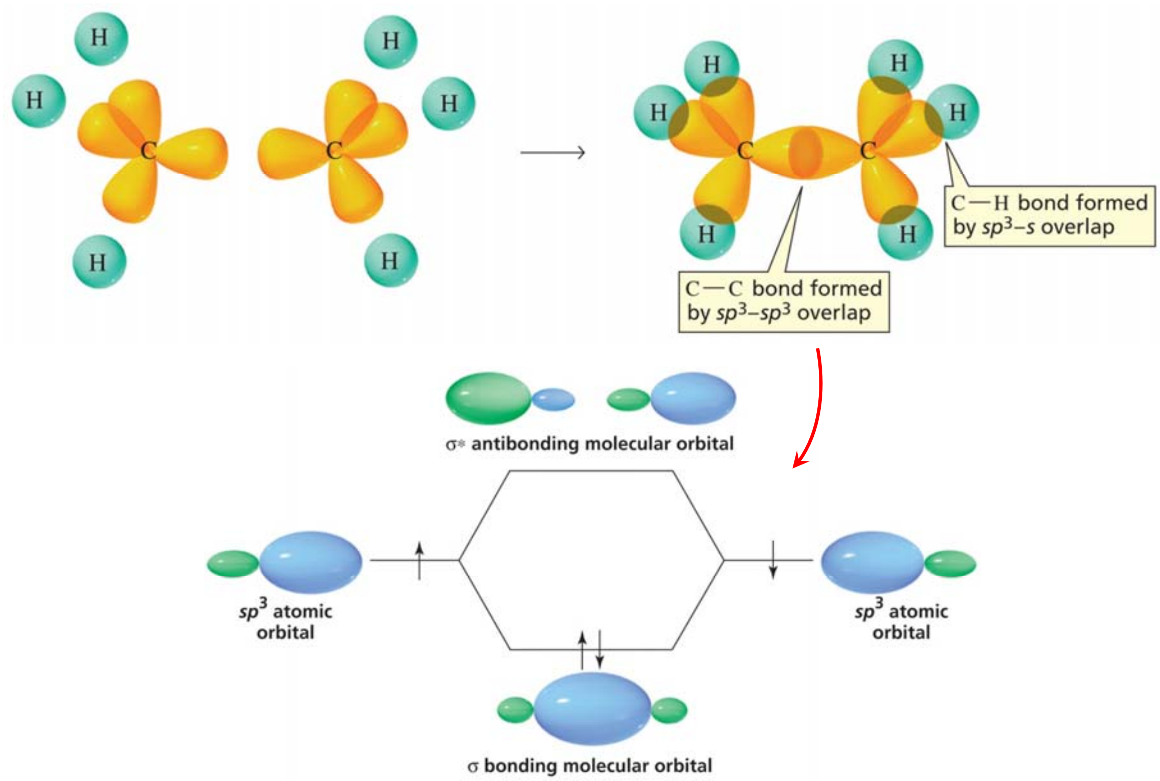
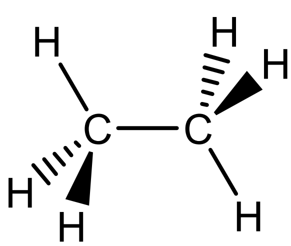
sp^3 Hybridization in Ethane (CH_3CH_3)

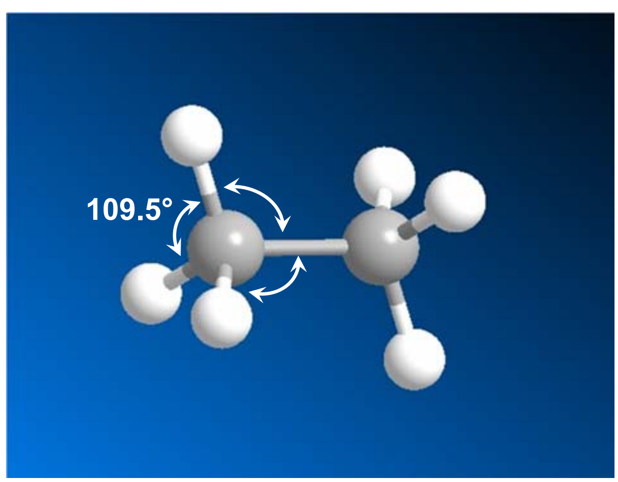


Geometry of Ethane (CH_3CH_3)

So, ethane is tetrahedral at both carbons.



All bond angles 109.5°

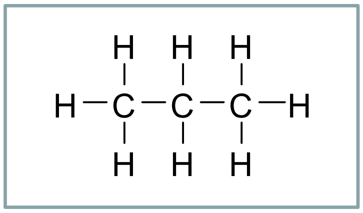


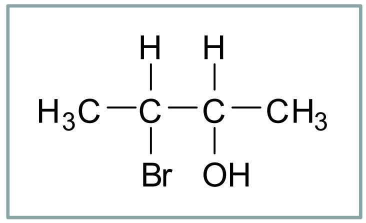
From ChemBio3D, free to UofM students; http://tinyurl.com/2301Office.

True for more complicated molecules too.

Wedge/Dash-Bond Drawings

How might you draw 3-D perspective for:

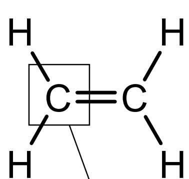




Three isomers of difluoropropane ($C_3H_6F_2$)

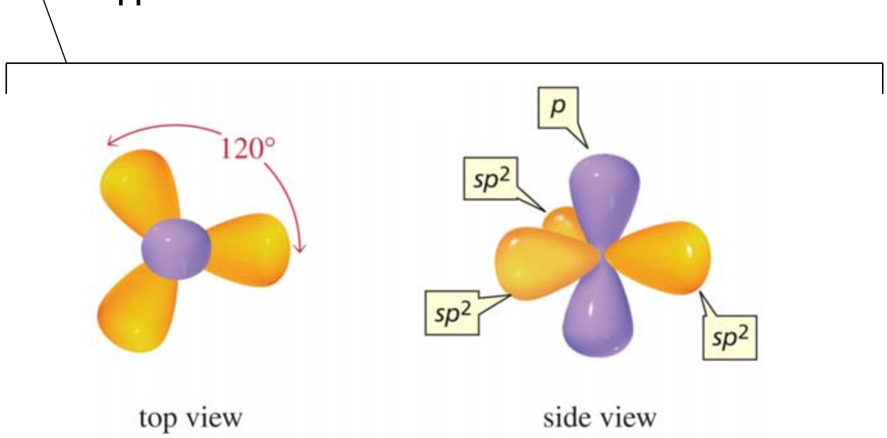
Draw all bonds and atoms.

Geometry of Ethene (CH_2CH_2)



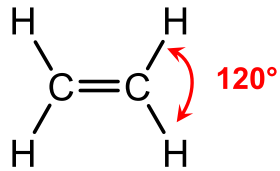
Each carbon has only 3 (σ) bonding partners;

So, carbons are s+p+p = sp^2 hybridized.

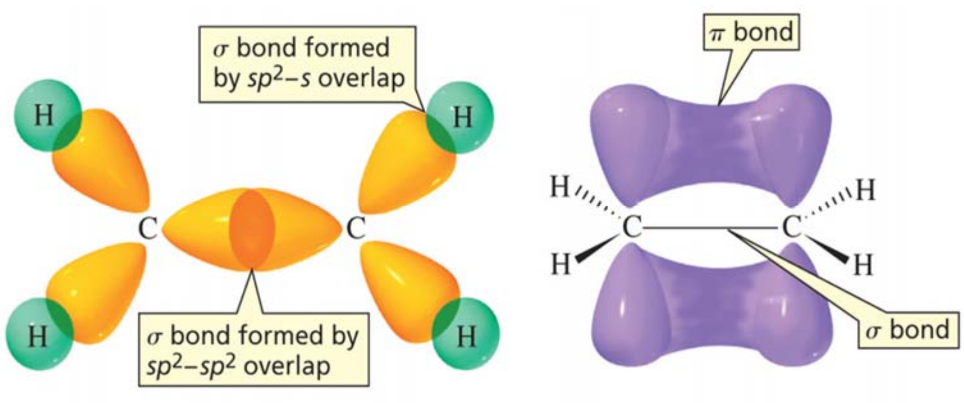


Only σ-bonding hybrid orbitals determine geometry by VSEPR.

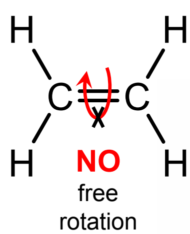
Geometry of Ethene (CH_2CH_2)

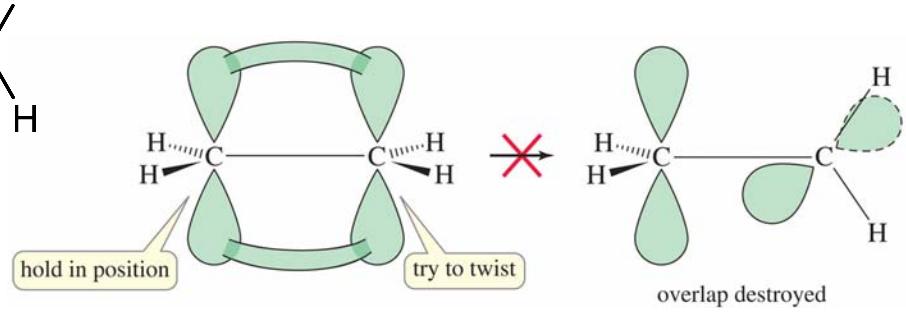


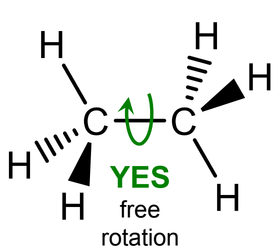
The two bonds of a double bond are not the same.

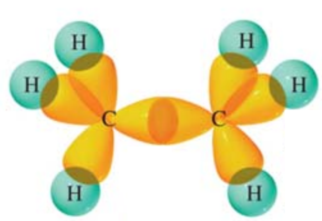


Free Rotation About Single Bonds, But Not Double Bonds



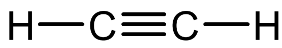






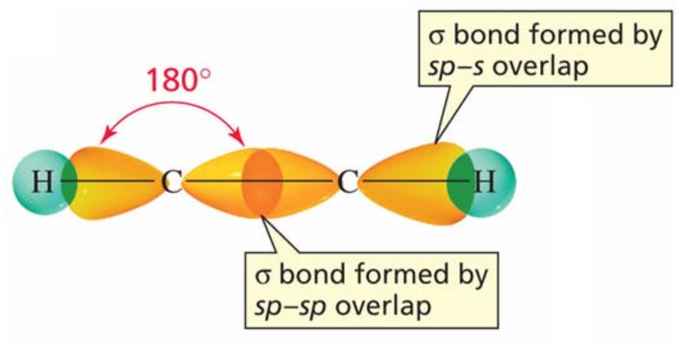
No orbital interactions that limit rotation.

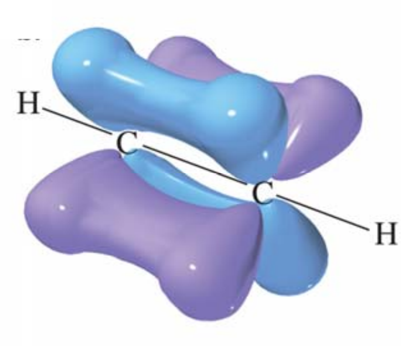
Geometry of Ethyne (HCCH)



Carbons are *sp*-hybridized;

Ethyne (acetylene) is linear.



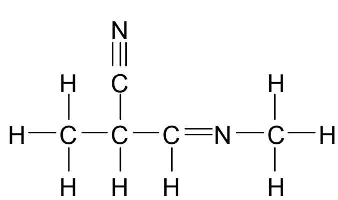


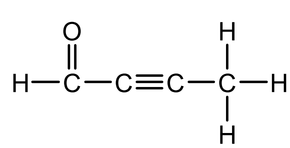
Interesting note: Rotation about triple bonds is actually okay;
Overlap between p orbitals is continuous enough through rotation.

Summary of Hybridization and Shape

Sum of σ-bonds and lone pairs	Hybridization	π-bonds	shape
4	sp^3	0	tetrahedral
3	sp^2	1	trigonal planar
2	sp	2	linear

So, for the two-dimensional molecule drawings below,
(i) Give the hybridization of all non-H atoms;
(ii) Re-draw the molecules to reflect a possible 3-D geometry.



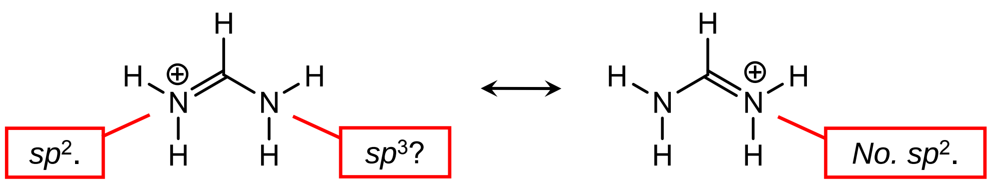


Including Resonance in Geometry

What if a molecule can be described by multiple good (major) resonance structures?

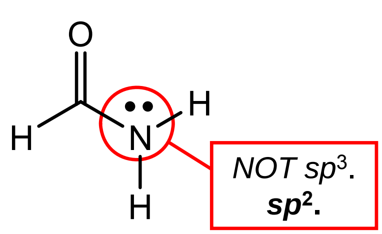
For each atom, the lowest hybridization state observed in major resonance structures is the correct one.

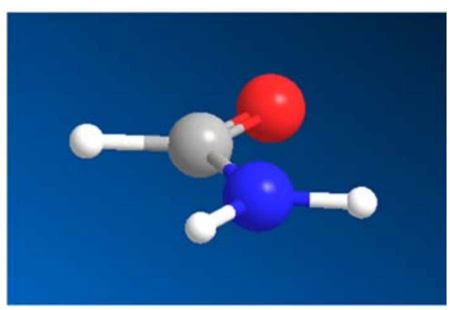
Example: *What is hybridization on nitrogen atoms?*



Answer: *Both are sp²*.

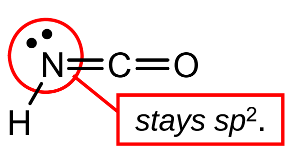
Nominally *sp*³-Hybridized Lone Pairs Adjacent to Multiple Bonds Switch to *p*

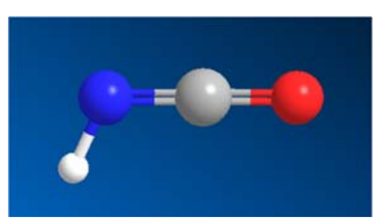




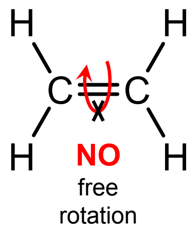
Lone pair occupies a p orbital, so it can mix with C-O π bond.

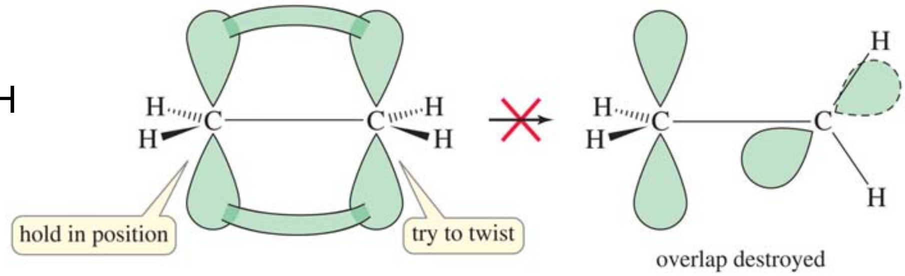
Oddly, this only works for nominally *sp*³ atoms.



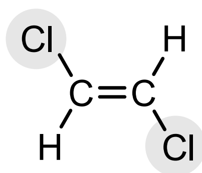


Last Week…

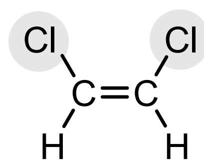




An important consequence:

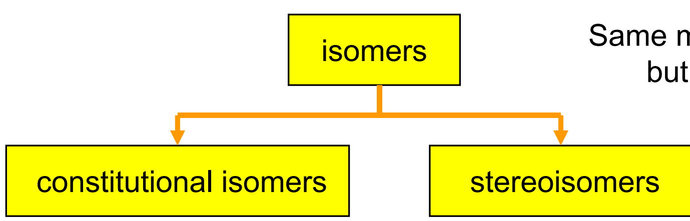


is not the same as



even though they're connected the same.

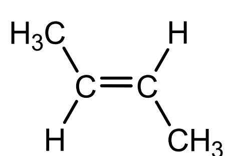
Stereochemistry and Isomerism



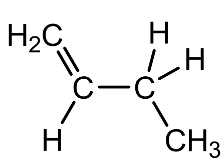
Same molecular formula, but not identical.

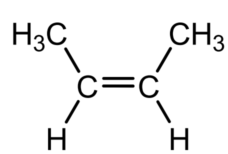
Different in the way their atoms are connected.

Same connectivity, but different spatial arrangement.



and *and*





are constitutional isomers. *are stereoisomers.*

Configurations and Conformations

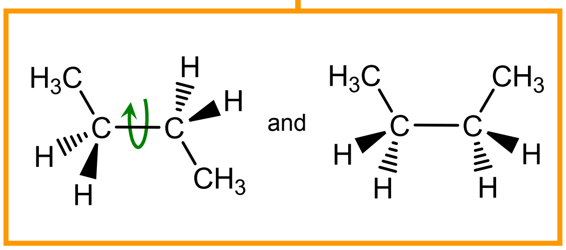
conformations
(e.g., rotation about single bonds)

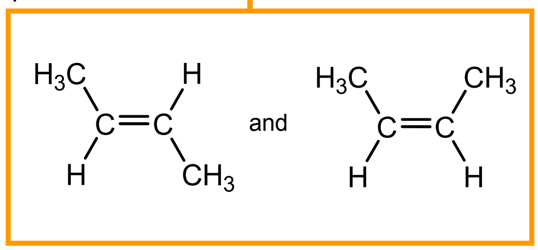
Interconvert rapidly at room temperature; cannot be separated

configurational isomers

Do not readily interconvert; can be isolated separately

for example,



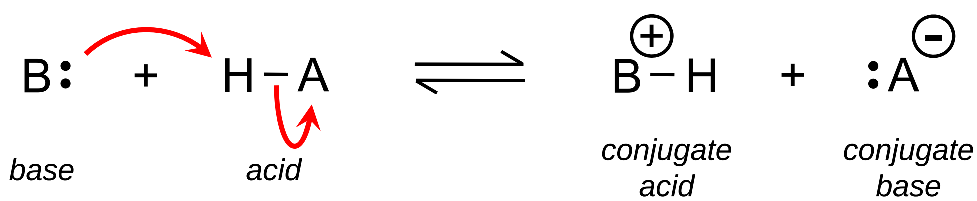


Electrons Drive Acid-Base Reactions

Lewis Base: An electron-pair donor.

Lewis Acid: An electron-pair acceptor.
(Here, also a proton donor.)

Organic chemists illustrate flow of electrons in reactions using curved arrows. (Sometimes called "electron pushing".)



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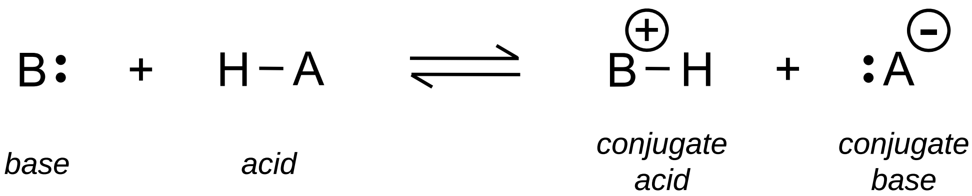

(Bronsted-Lowry acids & bases are defined in terms of protons. Almost the same.)