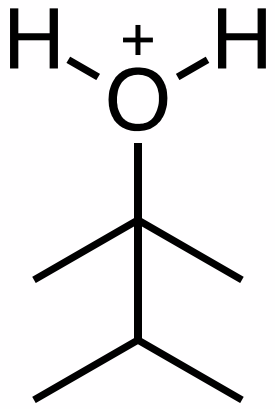
Objective 1

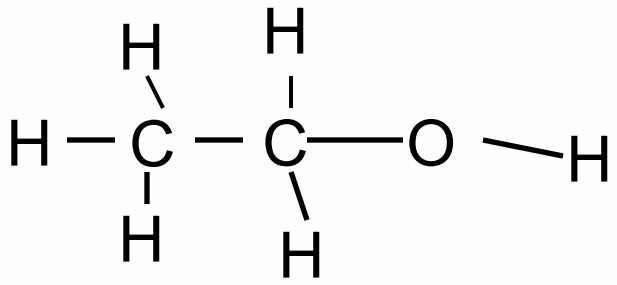
Represent organic molecules with chemical formulas, expanded formulas, Lewis structures, skeletal structures.
Determine shape (VSEPR), bond polarity, and molecule polarity.
Identify functional groups.

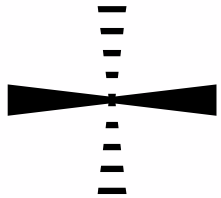
Learning Organic Chemistry

What do organic compounds look like?

How do I draw or represent organic compounds?







Bonding involves valence electrons.

How many valence electrons in:

1. C
2. H
3. O
4. N
5. P
6. S

(# of valence electrons = Group #)

A single bond consists of a bonding pair of electrons.

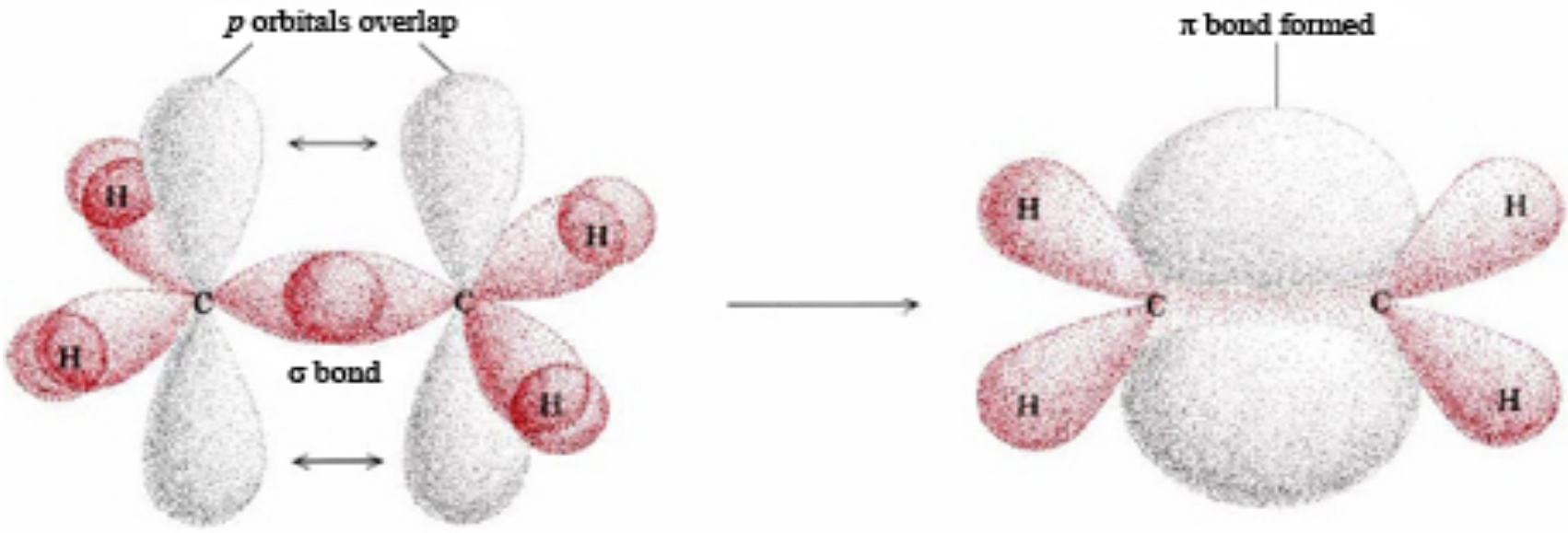
How does a bond form between two atoms?

How does a Bond form?

Bonding involves the overlap of orbitals

When two orbitals on the same axis overlap, a **sigma (σ) bond** forms.

When two orbital on parallel axes on the same plane overlap, a **pi (π) bond** forms.

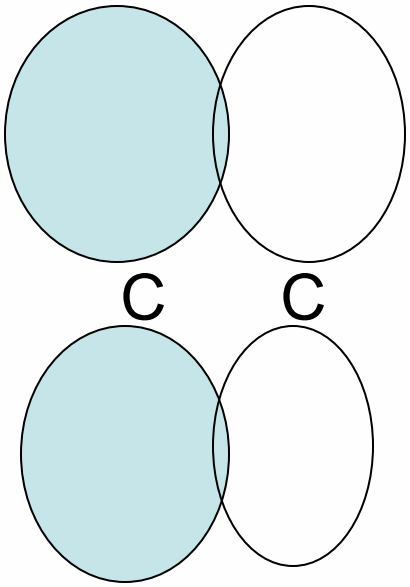


http://chemed.chem.wisc.edu/chempaths/GenChem-Textbook/Sigma-and-Pi-Bonds-858.html

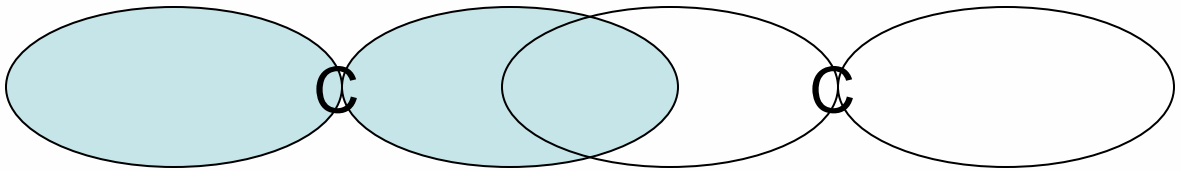
***How does a Bond form*?**

Bonding involves the overlap of orbitals.

Which bond is a sigma (σ) bond?
Which bond is a pi (π) bond?



A

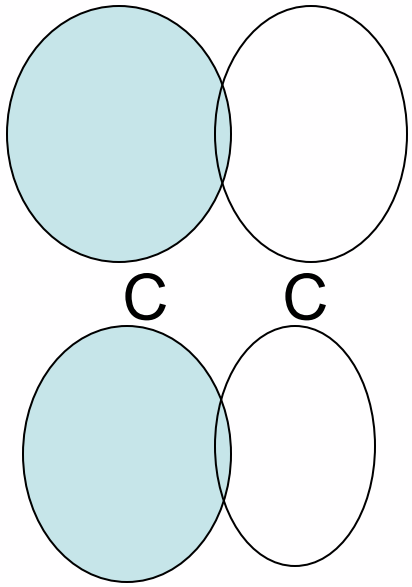


B

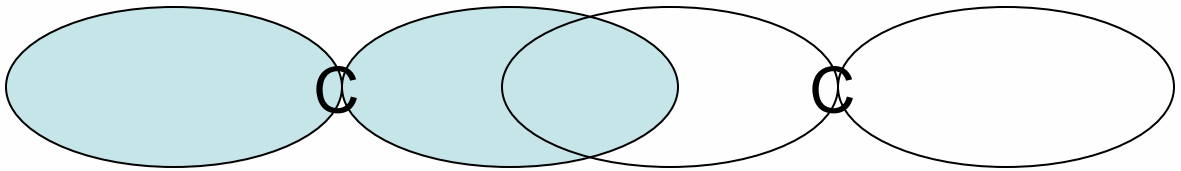
***How does a Bond form*?**

Bonding involves the overlap of orbitals.

Which bond is stronger, a σ bond or π bond? Why?



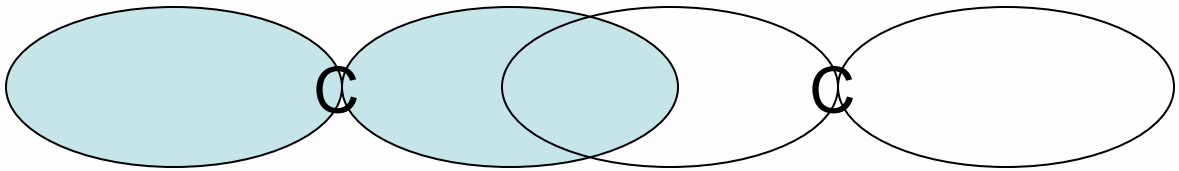
A



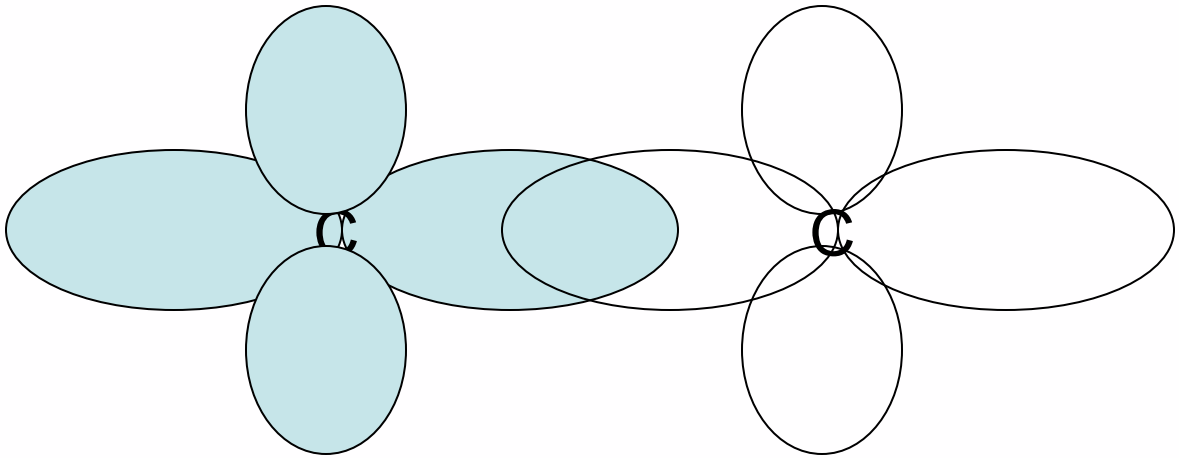
B

Carbon can form single bonds, double bonds, or triple bonds.

C-C **single** bond = 1 σ bond and 0 π bonds.

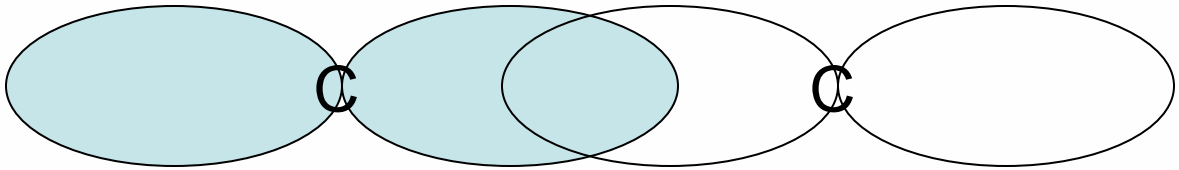


C-C **double** bond = 1 σ bond and 1 π bond.

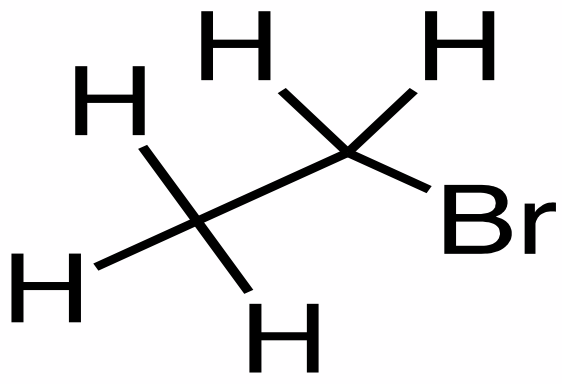


Carbon can form single bonds, double bonds, or triple bonds.

C-C **triple** bond = 1 σ bond and 2 π bonds. Draw in the π bonds.



Objective: determine bond polarity



Identify the polar bond(s) in this compound.

a. C-C b. C-H c. C-Br d. H-Br

For each polar bond, show the atom with the partial positive charge ($\delta+$) and the atom with the partial negative charge ($\delta-$).

What is a polar bond? What is a non-polar bond?_

$\delta+ \quad \delta-$

C - Br

Electronegativity determines bond polarity (who wins the "tug of war" for electrons in a bond).

http://biggirlbombshell.com/index.php/2012/06/tug-of-war/

Which atom is the most electronegative?

Compare C to H. Which atom is more electronegative?

Compare C to O. Which atom is more electronegative?

Compare O to H. Which atom is more electronegative?

Compare C to X. Which atom is more electronegative?

Functional Groups Are Small Groups of Atoms Within An Organic Compound

Hydrocarbons
Non-polar

Saturated

Alkanes
C-C

Unsaturated

Alkenes
C=C

Alkynes
C≡C

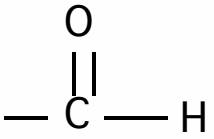
Aromatics

Groups that contain O
Polar

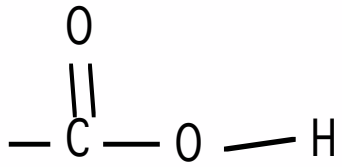
Alcohol
C-O-H

Ether
C-O-C

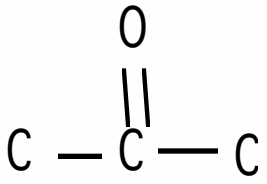
Aldehyde



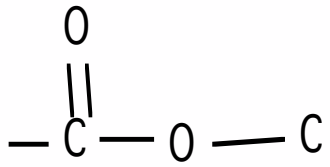
Acid



Ketone

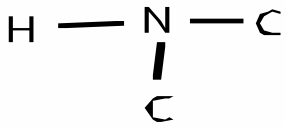


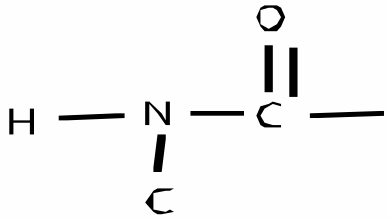
Ester



Other Groups: alkyl halides amines amides

X = F, Cl, Br, I





What does an Organic Molecule Look Like? Bonding ---> Structure ---> Shape

General Bonding Rules:

Carbon = 4 bonds and 0 lone pairs

Nitrogen = 3 bonds and 1 lone pair

Oxygen = 2 bonds and 2 lone pairs

Hydrogen = 1 bonds and 0 lone pairs

X (F, Cl, Br, I) = 1 bonds and 3 lone pairs

What does an Organic Molecule Look Like?

Bonding ---> Structure ---> Shape

Objective: Draw the Lewis structure of the following compounds.

C_2H_6

C_2H_5OH

C_2H_4

C_2H_2

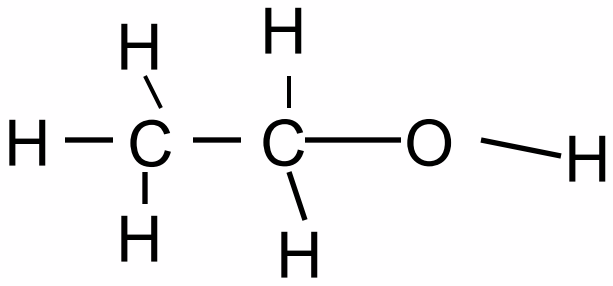
Identify the functional group in each compound.

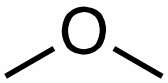
What does an Organic Molecule Look Like?

Bonding ---> Structure ---> Shape

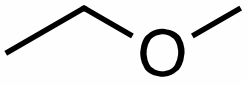
Objective: draw skeletal structure

Which skeletal structure (bond-line structure) matches the Lewis structure?

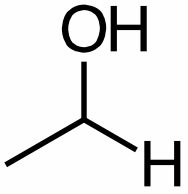




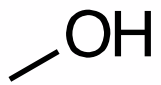
A



B



C

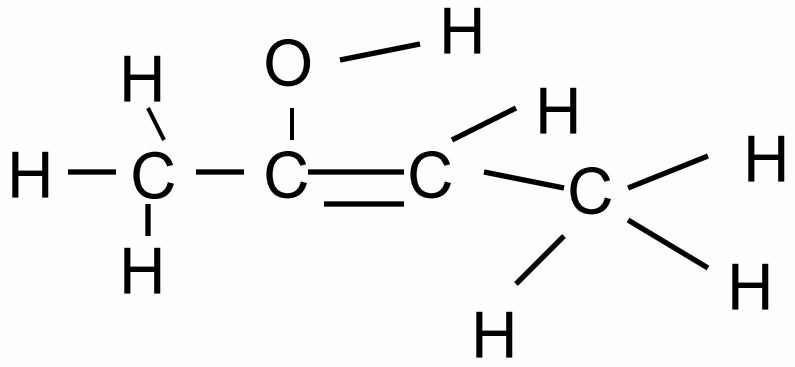


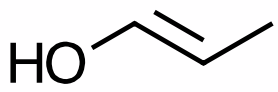
D

What does an Organic Molecule Look Like?

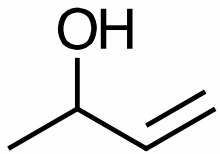
Bonding ---> Structure ---> Shape

Which skeletal structure (bond-line structure) matches the Lewis structure?

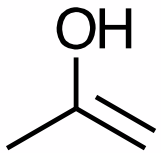




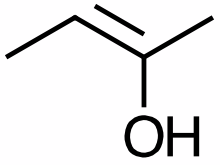
A



B



C



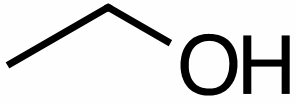
D

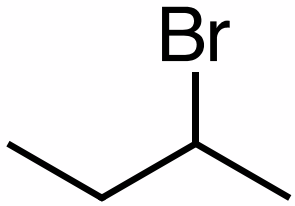
Objective: represent compounds by formula and structure

How do we represent organic compounds?

1. Chemical formula
2. Expanded formula
3. Lewis structure
4. Skeletal (bond-line) structure

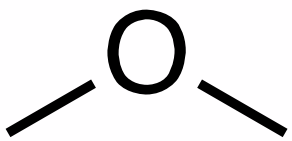
Are the compounds in each row the same or different???

C_2H_5OH CH_3CH_2OH 

$(CH_3)_3CBr$ C_4H_9Br 

Objective: represent compounds by formula and structure

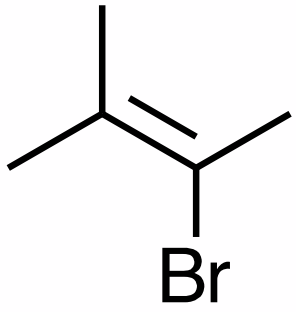
Which expanded formula matches the skeletal structure?



$CH_3CHOHCH_3$	$(CH_3)_2O$	CH_3CHO
A	B	C

Objective: represent compounds by formula and structure

Use numbers to write the expanded formula that matches the skeletal structure.



a. C

b. CH

c. CH_2

d. CH_3

e. Br

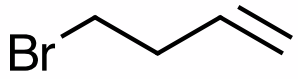
Enter your choices in your desired sequence.
If there are 2 or more of a group, include the number.

E.g., “dc2d” would be $CH_3(CH_2)_2CH_3$.

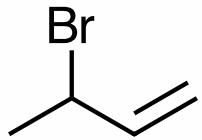
Objective: represent compounds by formula and structure

Which skeletal structure matches the expanded formula?

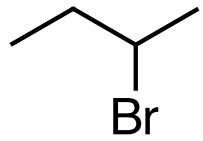
$CH_2CHCH_2CH_2Br$



A

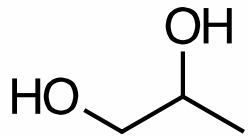


B

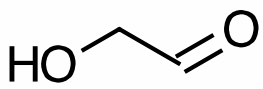


C

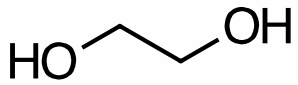
$CH_3CHOHCH_2OH$



A

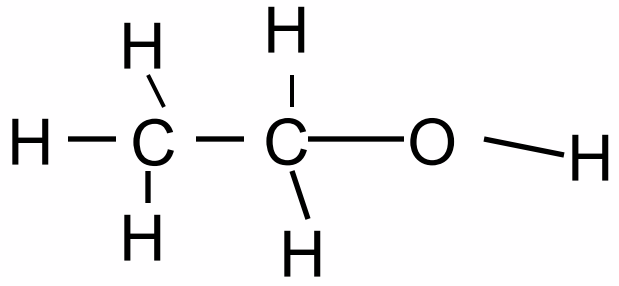


B



C

Determine the shape at each central atom:



C-1	linear	bent	trigonal planar	tetrahedral
C-2	linear	bent	trigonal planar	tetrahedral
O	linear	bent	trigonal planar	tetrahedral

VSEPR Theory (treat multiple bond as a single bond)

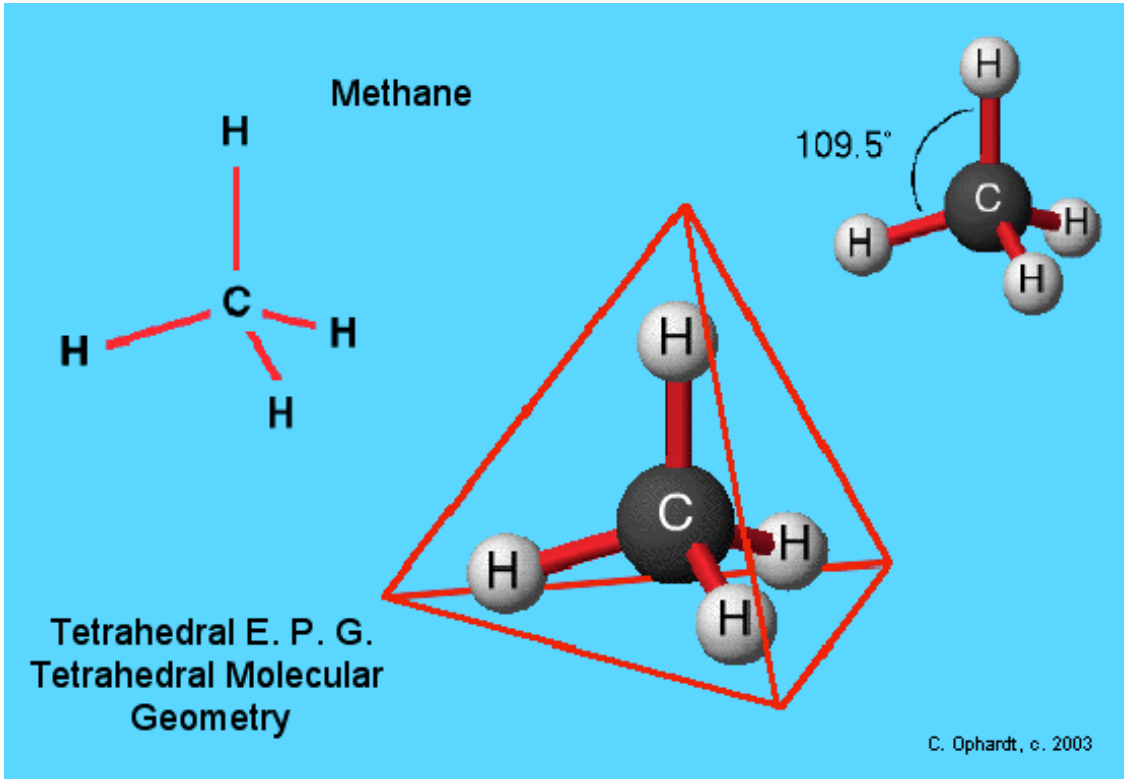
4 bonds and 0 lone pairs = Tetrahedral

3 bonds and 1 lone pair = Trigonal Pyramid

2 bonds and 2 lone pairs = Bent

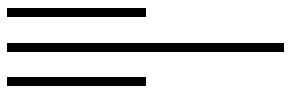
3 bonds and 0 lone pairs = Trigonal Planar

2 bonds and 0 lone pairs = Linear



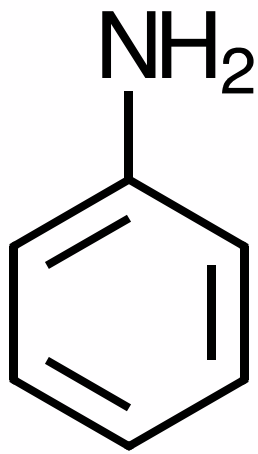
http://chemwiki.ucdavis.edu/Inorganic_Chemistry/Molecular_Geometry/Tetrahedral_Molecular_Geometry

Determine the shape at each central atom:



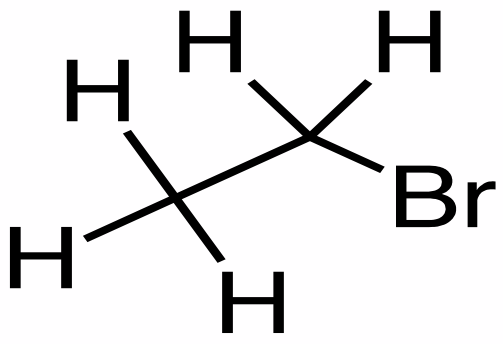
C-1	linear	bent	trigonal planar	tetrahedral
C-2	linear	bent	trigonal planar	tetrahedral
C-3	linear	bent	trigonal planar	tetrahedral

Determine the shape at each central atom:



C-1	linear	bent	trigonal planar	tetrahedral
C-2	linear	bent	trigonal planar	tetrahedral
N	linear	bent	trigonal planar	tetrahedral

Structure --> shape --> polarity --> properties, e.g., solubility

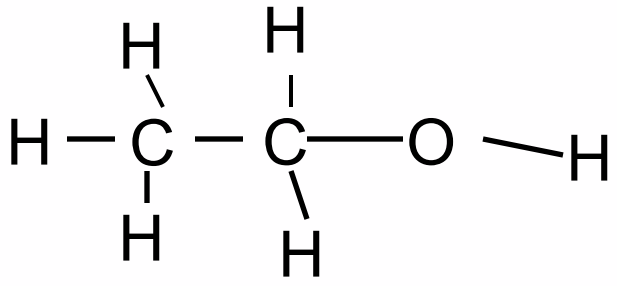


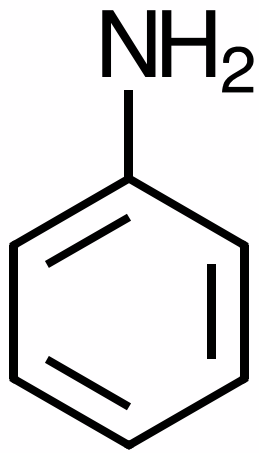
This molecule has polar bonds.

Is the molecule polar? YES NO

See chemagic.com - virtual molecular modeling kit

Polar or non-polar?



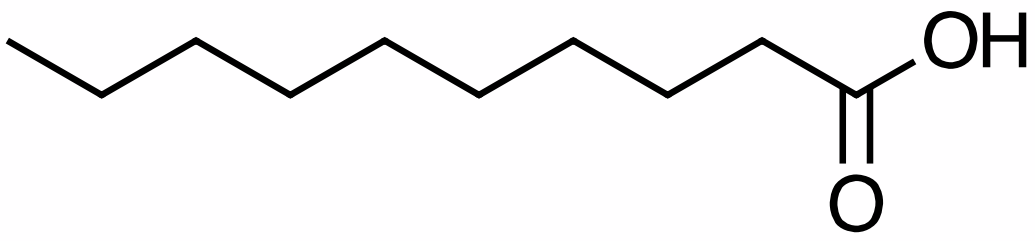


Polar or non-polar?

Groups that contain O are _____.

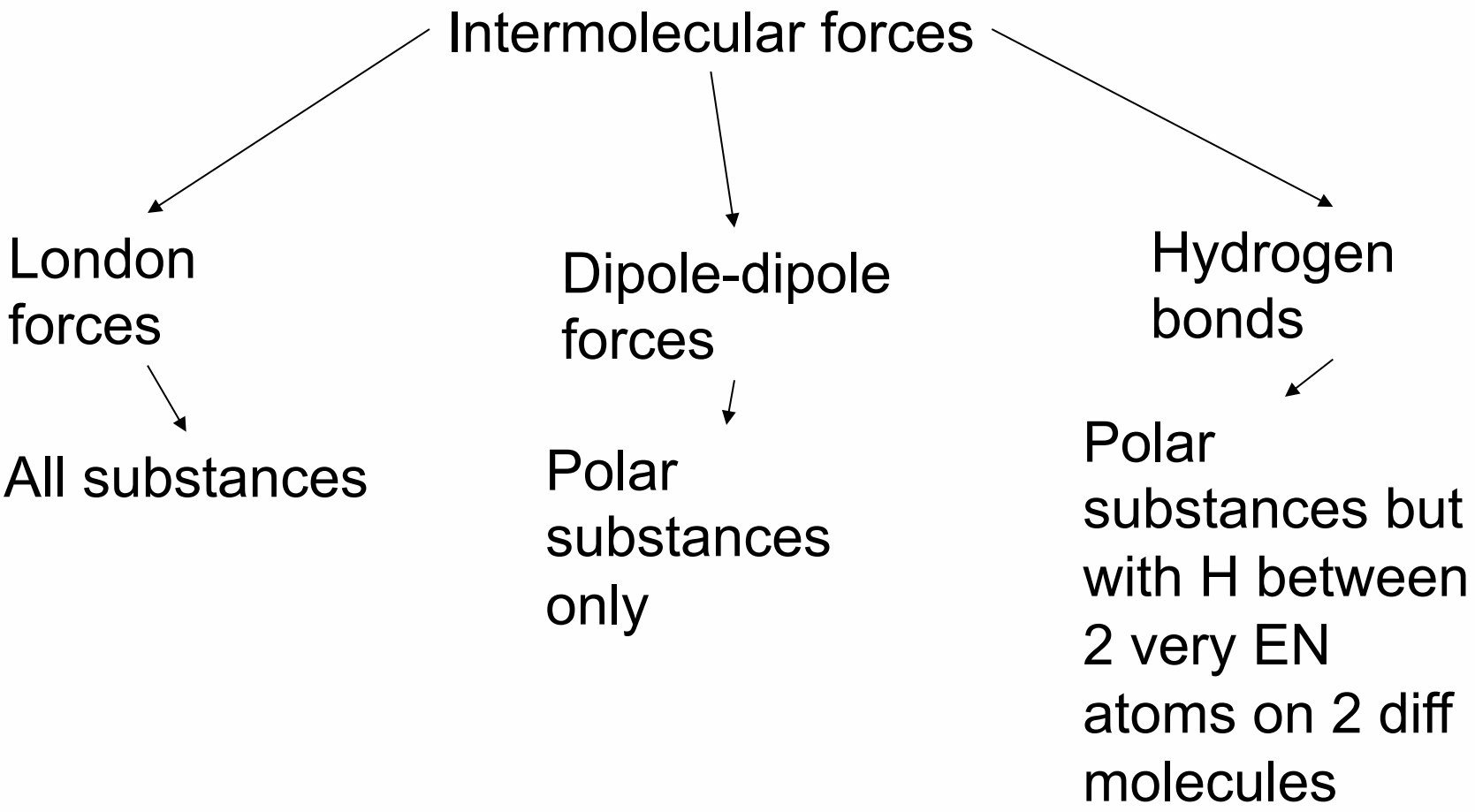
Hydrocarbons (saturated and unsaturated) are _____.

Fatty acids have an acid group connected to a hydrocarbon chain. Why are fatty acids insoluble in water?

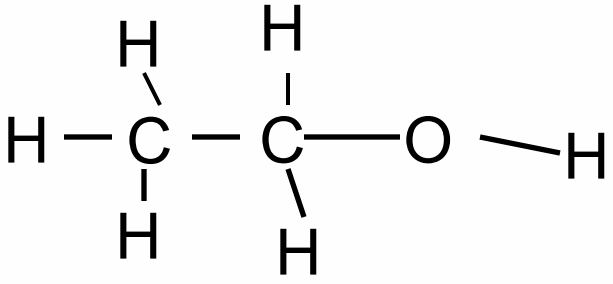


INTERMOLECULAR Forces are ***<u>WEAK</u>*** compared to ***INTERATOMIC*** Forces

Give one example of an interatomic force.

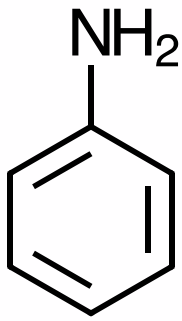


Determine the IM forces in each compound



London dipole-dipole H bonds

London dipole-dipole H bonds



London dipole-dipole H bonds

B.p. and m.p. depend on IM forces.

Stronger IM force means _____ (higher or lower?) b.p.

Using IM forces, explain why ethane has a lower b.p. than ethanol.

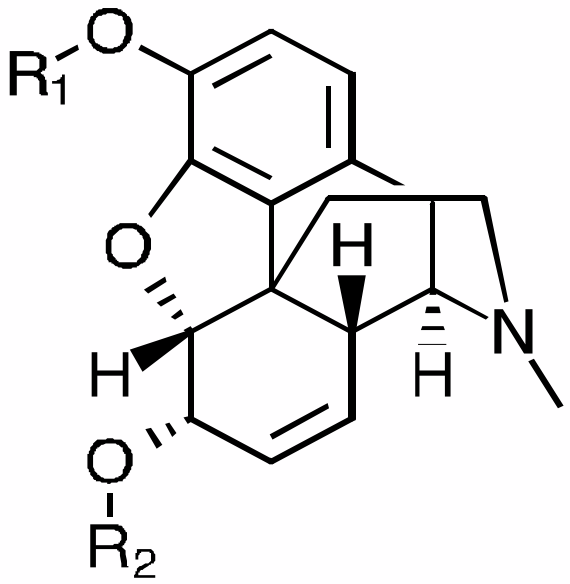
Lipids are _____ and are _____ in water.

Blood is mostly water. How are lipids transported through blood?

How can you make a compound that is insoluble in water more soluble?

Structure, Shape, and IM Forces Determine Drug Interaction
Drug Receptor and Pharmacophore

Morphine - narcotic (analgesic, hypnotic euphoriant)



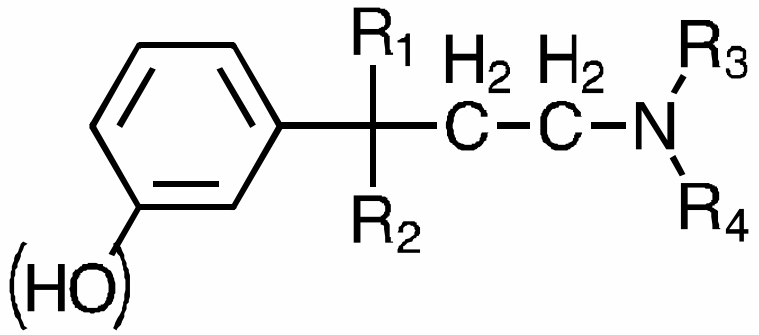
Morphine	$R_1 = H = R_2$
Codeine	$R_1 = CH_3$
	$R_2 = H$
Heroin	$R_1 = CH_3CO-$
	$R_2 = CH_3CO-$

Is this molecule flat (planar)?

See chemagic.com

"Morphine Rule" - 4 structural features of strong narcotic analgesics

1. Ring
2. Quaternary C
3. Ethylene bridge
4. 3° amine

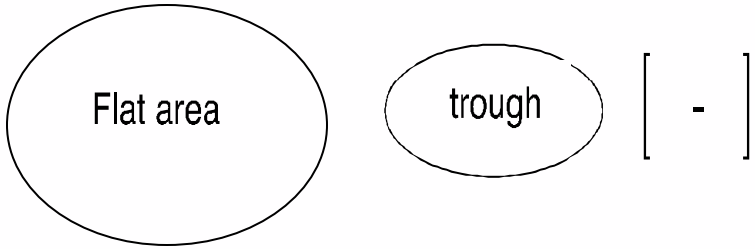


3 essential receptor features:

1. Flat area that binds to ring, probably by van der Waals interaction.
2. an anionic site that attracts the 3° amine. Amine is usually protonated and (+) charged. See pH and pK of amine.

$$NR_3 + H^+ \rightarrow NR_3H^+$$

3. a suitably oriented trough between ring and amine to accommodate $-CH_2-CH_2-$ bridge.



Methane = CH_4. *Why is C tetrahedral* ?

Draw the ground state valence electron configuration of **CARBON** (CHM 1A)

Based on this ground state configuration, how many bonds form to C?

How do 4 bonds form to C?

What is the shape based on the directions of the s and p orbitals?

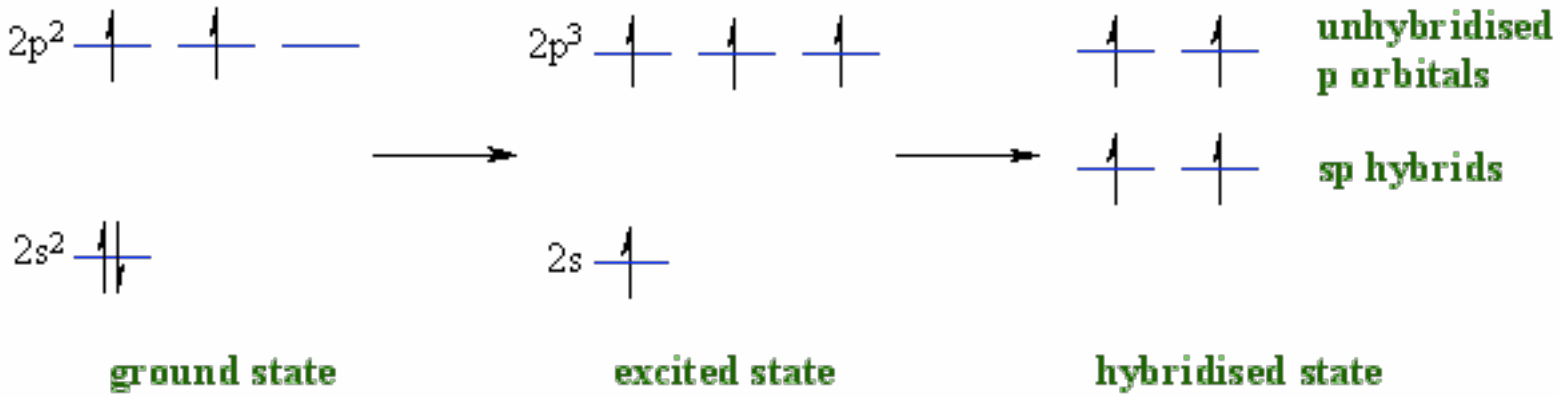
Valence Bond Theory and Molecular Orbital Theory are the Two Main Bonding Theories

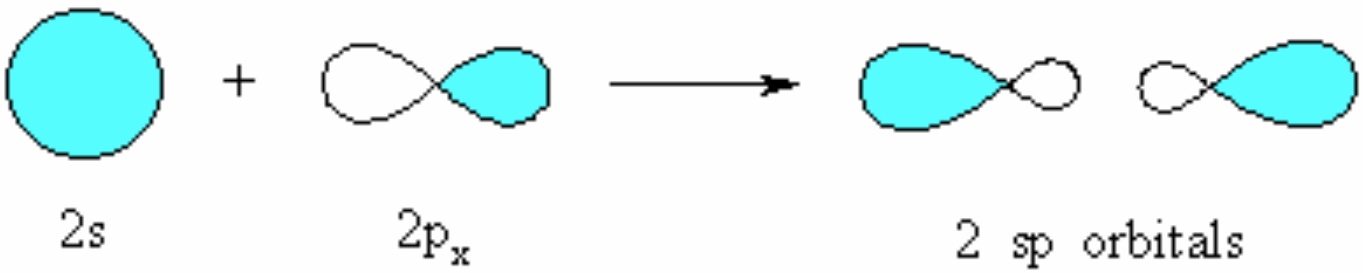
Valence Bond Theory	Molecular Orbital Theory
Two orbitals in the same atom combine together to form hybrid orbitals.	Two orbitals in different atoms combine together to form molecular orbitals.
Localized electrons	Delocalized electrons
Structure and shape	Magnetism and color

We will focus on Valence Bond Theory in Chem 12.

A hybrid orbital forms when one s orbital combines with 1, 2, or 3 p orbital(s) from the same atom (usually C).

one s orbital + one p orbital --> two sp hybrid orbitals

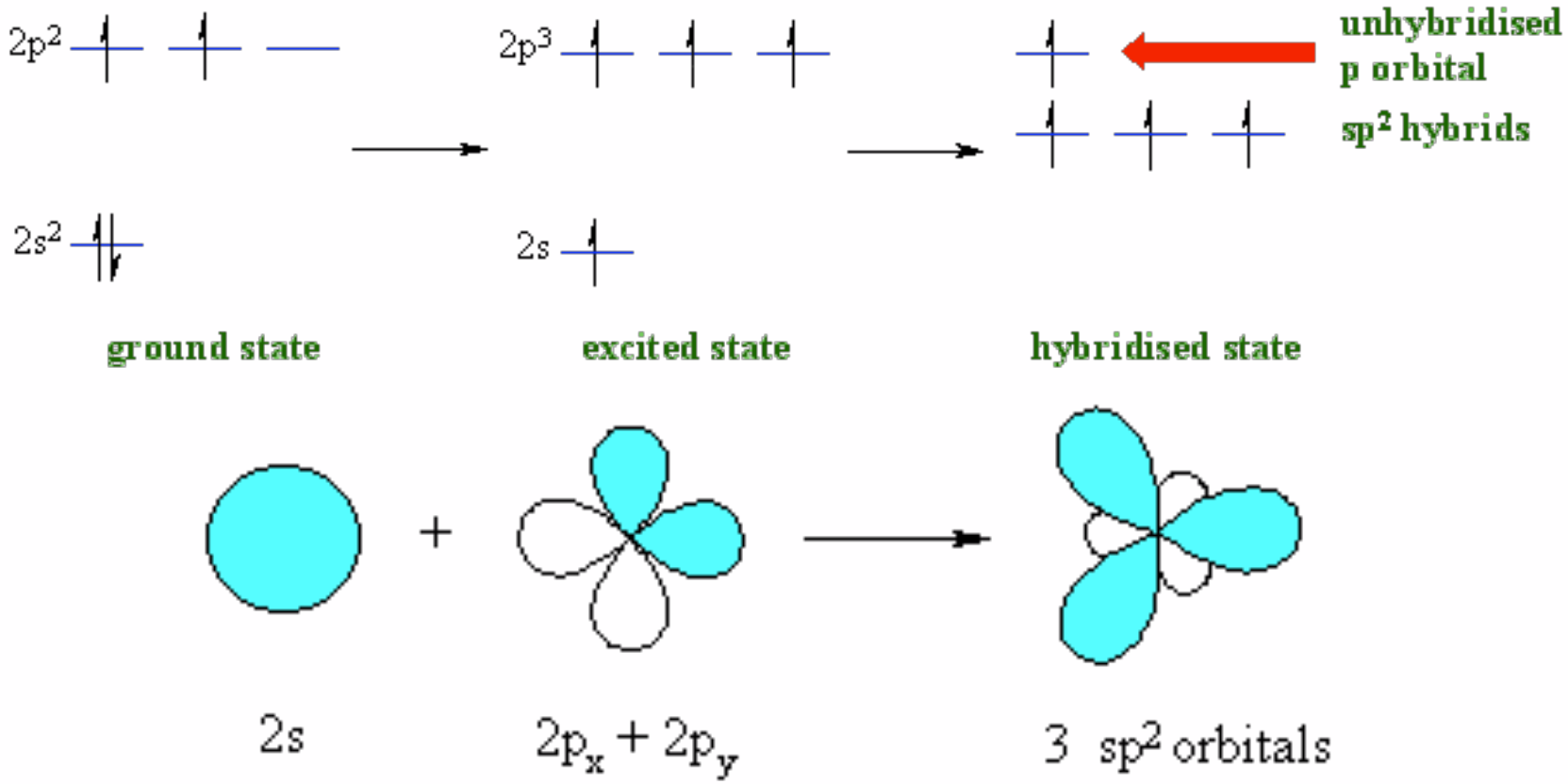




http://www.chem.ucalgary.ca/courses/351/Carey5th/Ch02/ch2-3-3.html

A hybrid orbital forms when one s orbital combines with 1, 2, or 3 p orbital(s) from the same atom (usually C).

one s orbital + two p orbital --> three sp^2 hybrid orbitals



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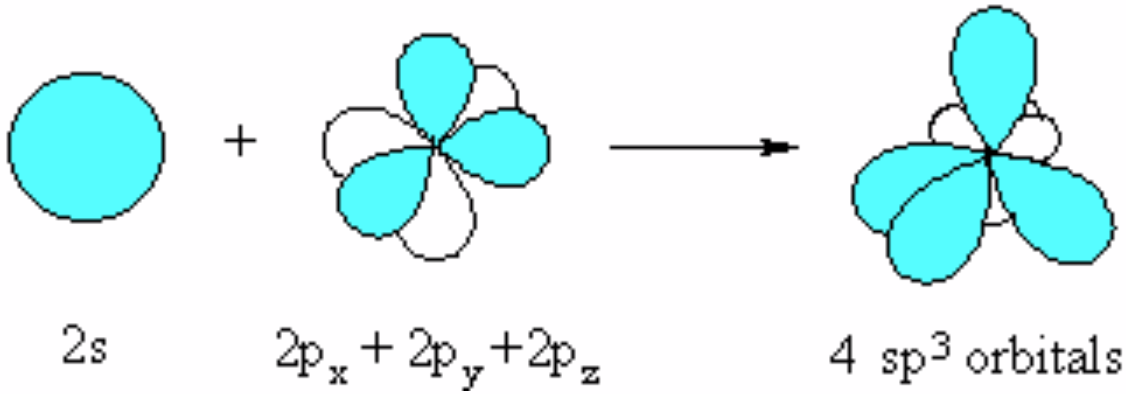
A hybrid orbital forms when one s orbital combines with 1, 2, or 3 p orbital(s) from the same atom (usually C).

one s orbital + three p orbital --> four sp^3 hybrid orbitals

Draw the orbital diagram that show how sp^3 hybrid orbitals form.



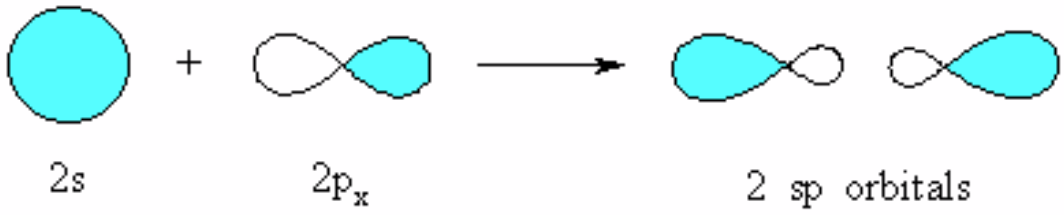
http://www.chem.ucalgary.ca/courses/351/Carey5th/Ch02/ch2-3-1.html

Hybrid Orbitals Explain SHAPE

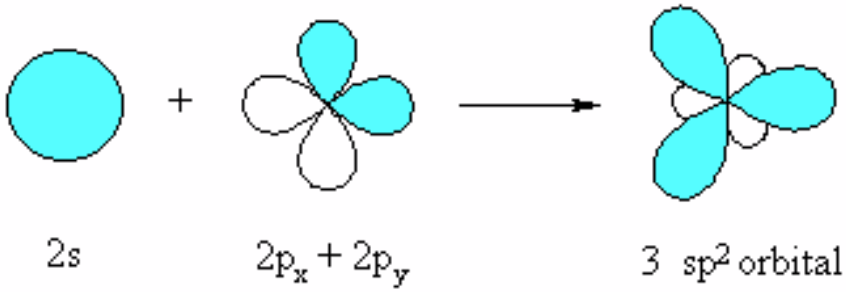
Each hybrid orbital points in a specific direction(s) and explains shape.

Animation: http://www.chem.ucalgary.ca/courses/351/Carey5th/Ch02/ch2-3-1.html

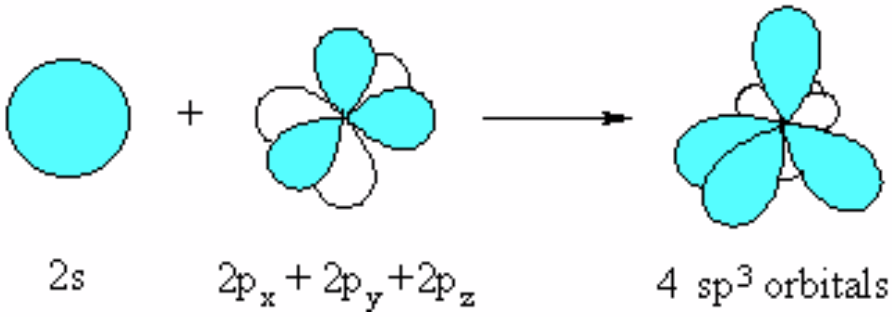
sp hybrid orbitals point in opposite directions --> linear



sp^2 hybrid orbitals point to the corners of a triangle --> trigonal planar



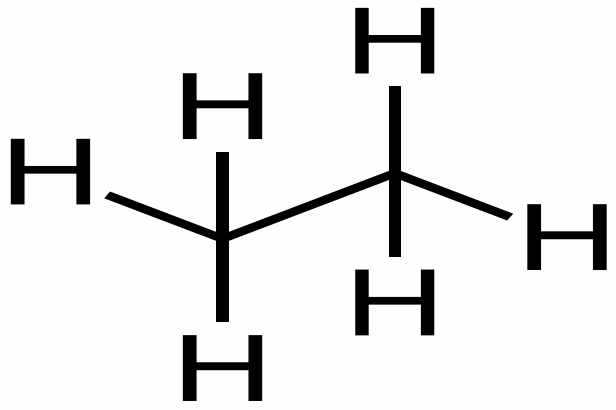
sp^3 hybrid orbitals point to the corners of a tetrahedron --> tetrahedral



Hybridization Explains Bonding and Shape

Objective: ID orbitals involved in bond

E.g., C_2H_6



C = 4 single bonds = tetrahedral --> sp^3 hybrid orbitals

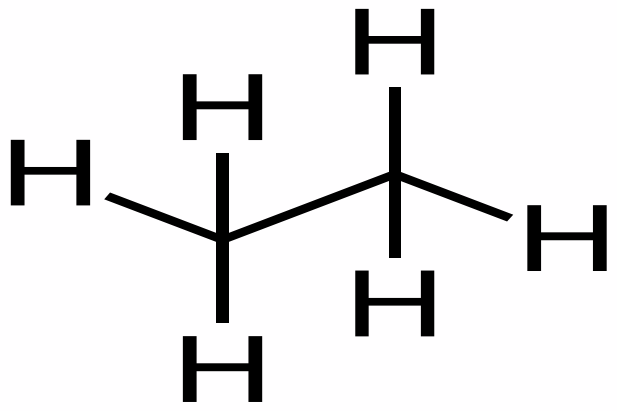
C1-C2 σ bond forms between _____ orbitals on each C

a. s and s
b. s and p
c. sp and sp^2
d. s and sp^2
e. sp^2 and sp^3
f. sp^3 and sp^3

Hybridization Explains Bonding and Shape

Objective: ID orbitals involved in bond

E.g., C_2H_6



C = 4 single bonds = tetrahedral --> sp^3 hybrid orbitals

C-H σ bond forms between ___ orbital on C and ____ orbital on H. Enter your choices in your desired sequence.

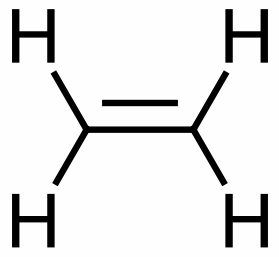
a. s
b. p
c. sp
d. sp^2
e. sp^3
f. sp^4

Hybridization Explains Bonding and Shape

Objective: ID orbitals involved in bond

Hybrid orbitals on Carbon form σ bonds.
p orbitals on Carbon form π bonds.

Describe the bonding in C_2H_4
C = 2 single bonds, 1 double bond
= trigonal planar --> sp^2 hybrid orbitals



C1-C2 σ bond forms between _____ orbitals on each C

C1-C2 π bond forms between _____ orbitals on each C

H-C2 ___ bond forms between _____ orbital on H and _____ orbital on C2.

Fill in the blanks in the table:

Electron geometry	Bond angle	VB hybridi-zation	Bond types (σ or π)	% s character	% p character
Tetrahe-dral					
Trigonal planar					
Linear					

Structure/Shape/Hybridization Tells Us:

1. What an organic compound looks like.
2. Helps us explain bond strength and reactivity.

Compare ethane (C_2H_6), ethylene (C_2H_4), and acetylene (C_2H_2),
Which C-C bond is the strongest? Give reasons.
Which C-H bond is the strongest? Give reasons.
(see IR table on Slide 46)

How do these molecules look the same?
How do these molecules look different?
Do you think electrons in σ bonds or π bonds are more likely to react?

Bigger Orbital Overlap Means Stronger Bond

- A _____ (stronger or weaker) bond will have _____ (more or less) s character in the bonding orbital.

- In general, a weak bond is _____ (more or less) reactive than a strong bond.

- A C-C single bond is unreactive.

- The π bond in a C-C double bond or triple bond is reactive.