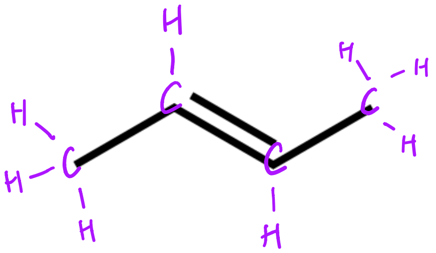
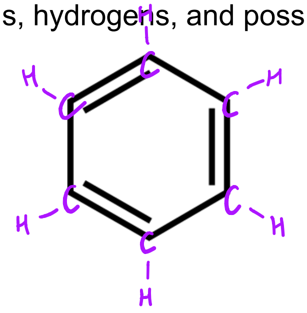
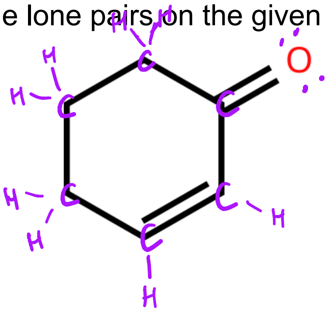
Session 2 Worksheet

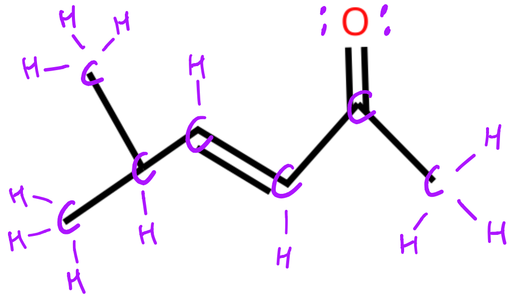
In organic chemistry, we mainly use bond line structure to represent compounds, however, converting bond line to condensed formula (and vice versa) is important to understand and know how to do.

First, start with labelling all carbons, hydrogens, and possible lone pairs on the given structures:



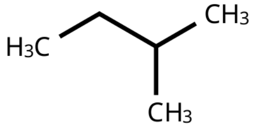
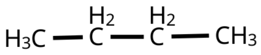
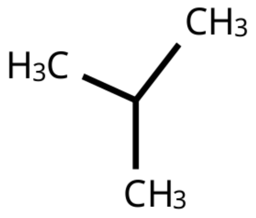






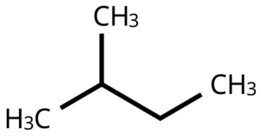
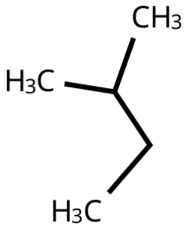
Constitutional Isomers

What is the relationship of these molecules? Different, Same, or Constitutional Isomers?

C_4H_{10}	
 $H_3C-\overset{H_2}{C}-\overset{H_2}{C}-CH_3$	

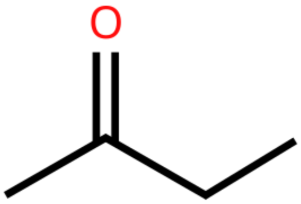
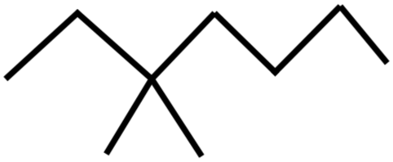
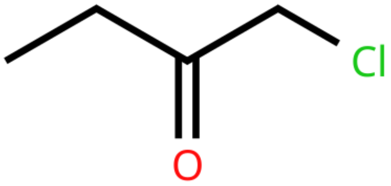
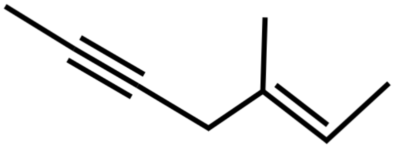
Different

Constitutional Isomers

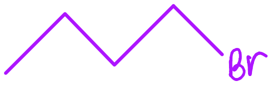
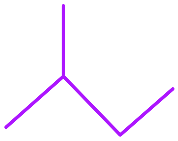
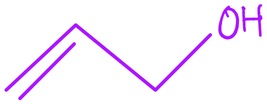
	

Same

Write the condensed formula given the structure:

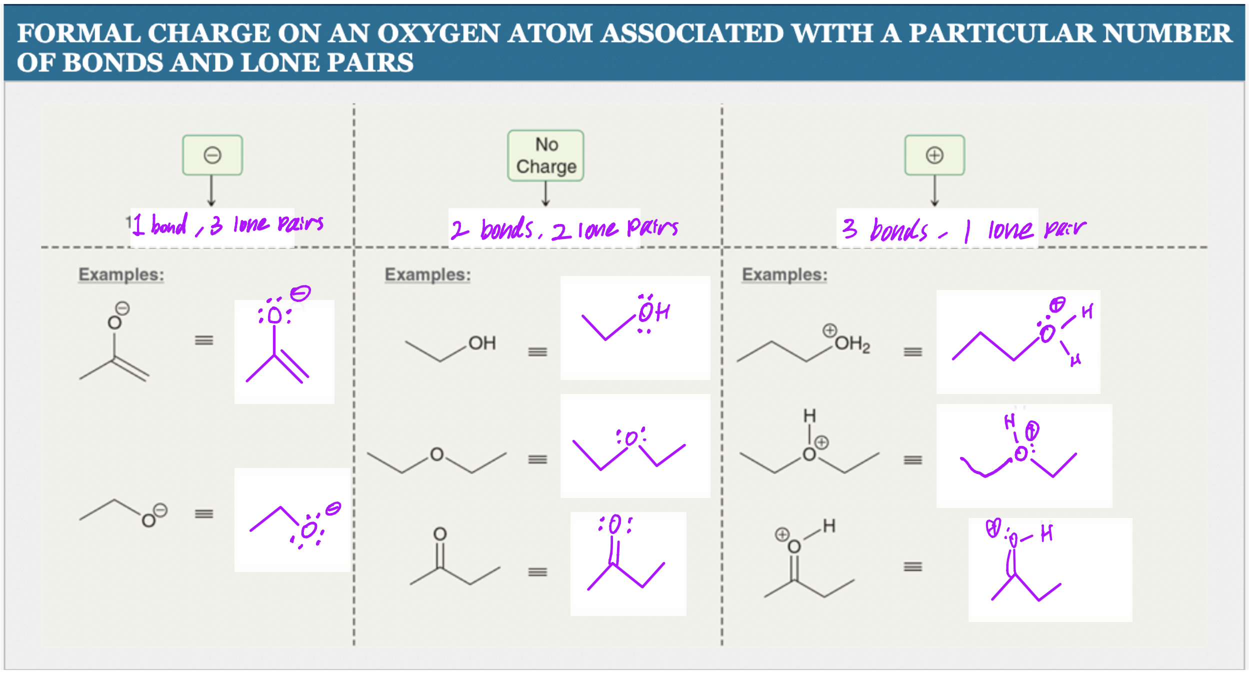
	$CH_3COCH_2CH_3$
	$CH_3CH_2C(CH_3)_2(CH_2)_3CH_3$
	$CH_3CH_2COCH_2Cl$
	$CH_3CCCH_2C(CH_3)CHCH_3$

Write the structure given the condensed formula:

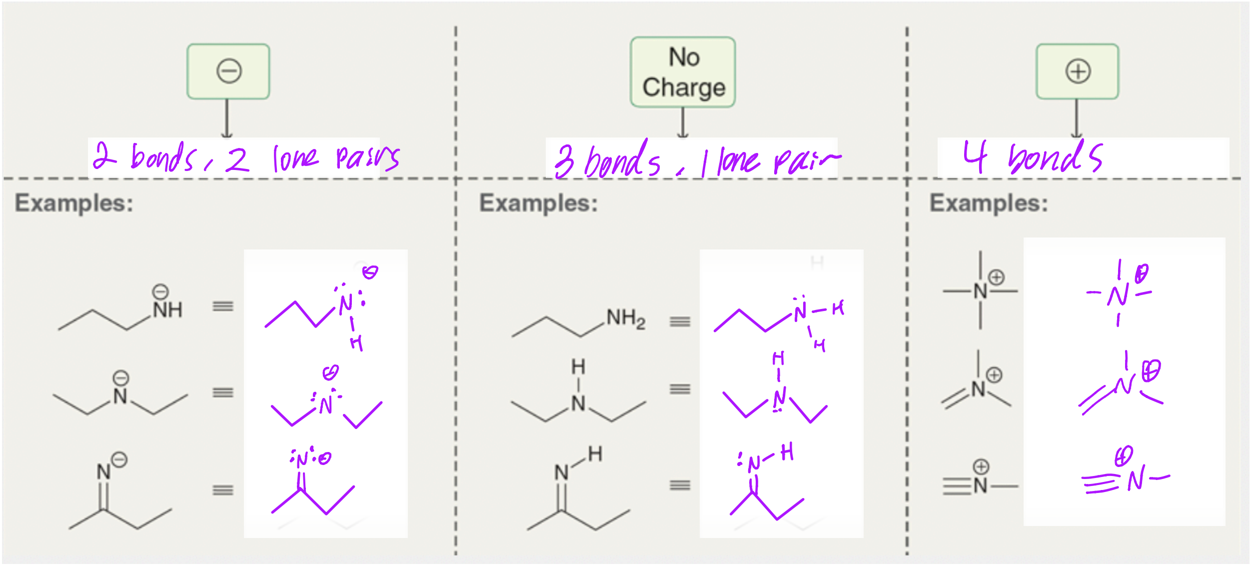
$CH_3CH_2CH_2CH_2Br$	
$CH_3CH(CH_3)CH_2CH_3$	
CH_2CHCH_2OH	

Summary of formal charges:

Oxygen Summary:



Nitrogen Summary:

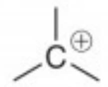


Introducing Carbocations:

- ⊕ charged carbons
- Important intermediate for reactions

Recall: carbon is tetravalent

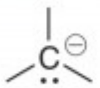
Carbocation:



Carbocation

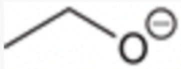
Carbanion:

negative charge

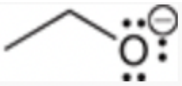


Carbanion

You do not have to write lone pairs if you don't want to, however, you MUST include a formal charge (if applicable)



is the same as



Resonance:

- Shows distribution of charge

Resonance structures:

- Ways these charges can appear

We represent resonance structures with Brackets and double sided arrows

Note: the resonance structures are not switching back and forth! The hybrid is a mixture of both structures

Delocalization:

- e^- in a molecule that are not associated with a bond
  - can be "moved"

Resonance Stabilization:

- How certain molecules can stabilize with charges
- resonance = stability

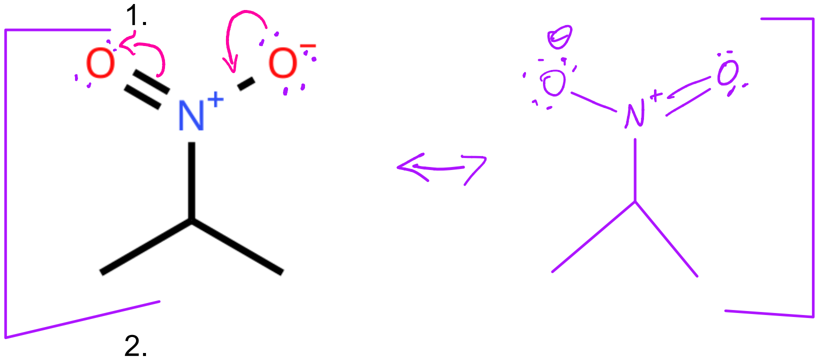
Curved Arrows:

Shows e^- as if they are moving, but they're not

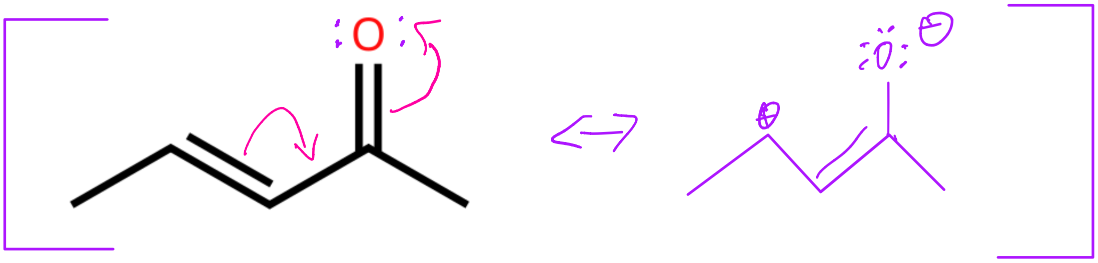
Use a double-barbed arrow, single-barbed arrows show the movement of radicals (single e-)

Resonance Demonstration:

1.



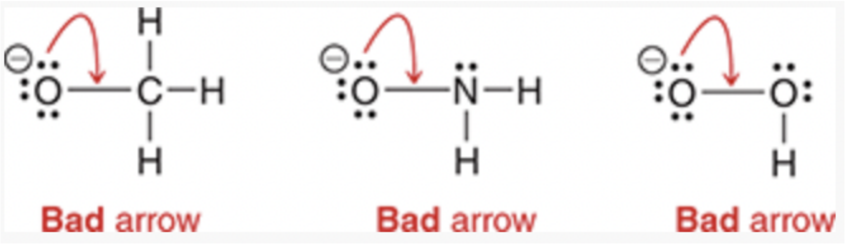
2.



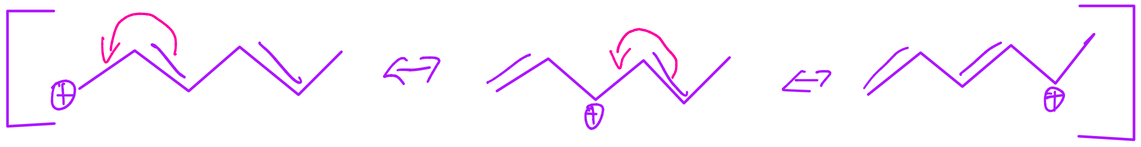
NEVER DO THIS IN RESONANCE:

1. break single bonds

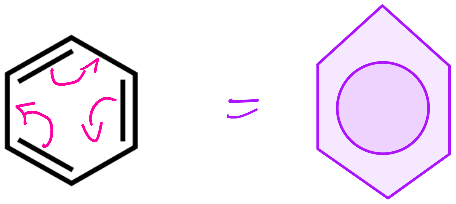
2. over fill the octet



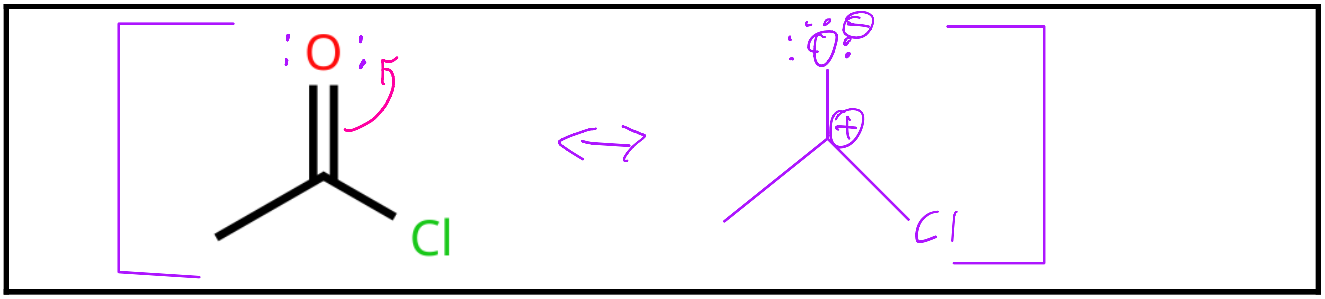
More than 1 resonance structure:

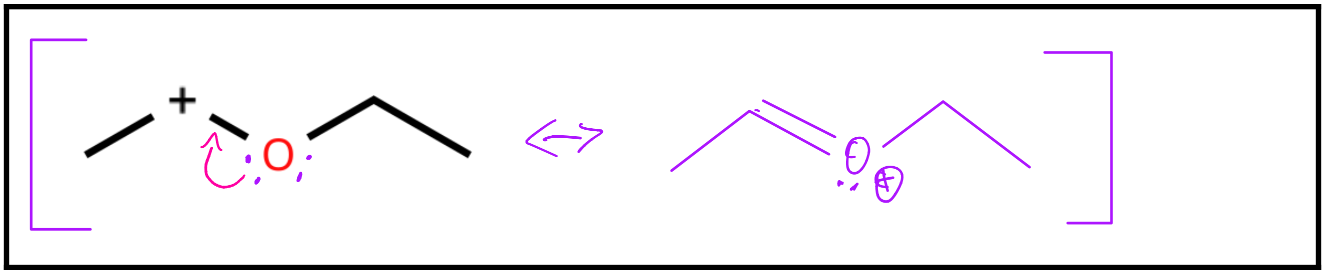


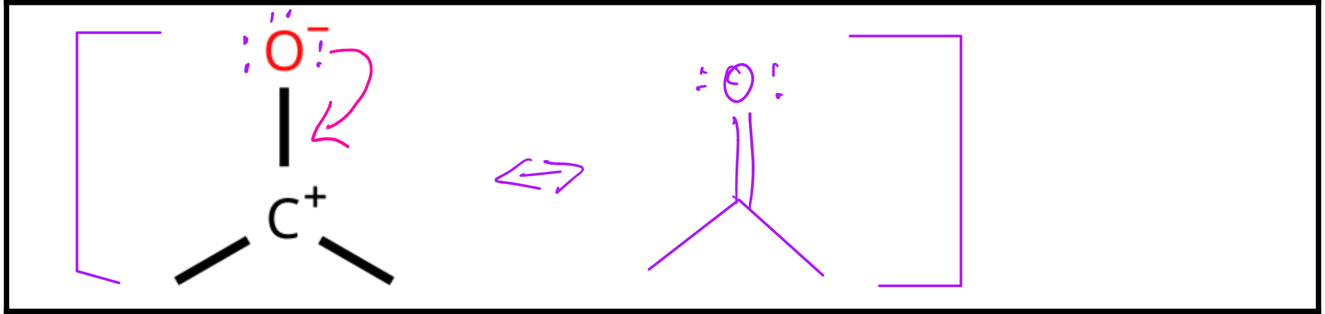
Conjugated pi bonds in a ring:

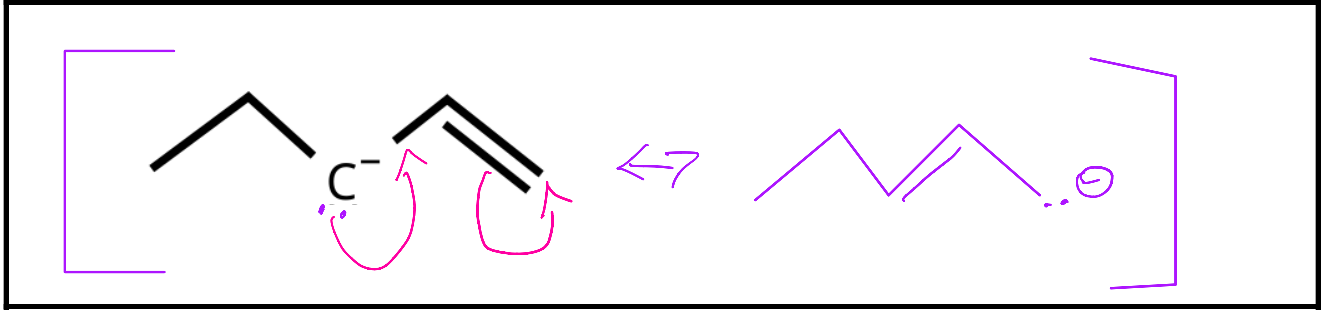


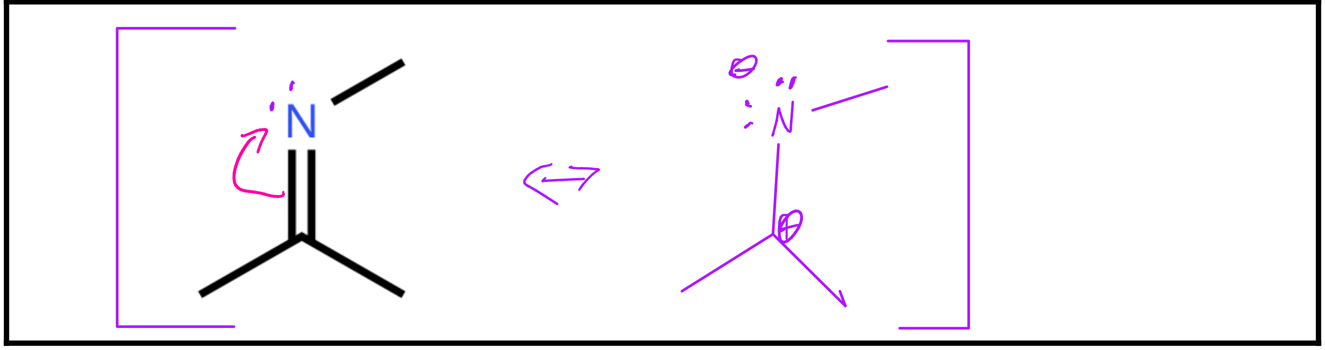
Practice :) (Draw all lone pairs 1st)




+
O
⊖
⊕

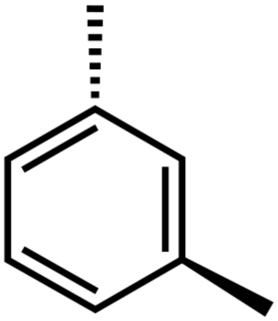

O⁻
C⁺
⊖


C⁻
⊖


N
⊖
N
⊕

Wedges and Dashes:

When thinking about molecules in a 3D plane, we use dashes to represent the substituent going behind the page, and wedges to represent the substituent coming out of the page



Quantum Mechanics

Molecular orbitals

- Represents the region of space where one or two electrons of a molecule are likely to be found
- Have a wave-like behavior with + and − lobes

Remember

The +/- lobes are not an indicator of charge, simply, they are an illustration of displacement

Bonding MO:

- Result of constructive interference
- forms bonds
- lower in energy

Anti-bonding MO:

- Result of destructive interference
- does not form bonds
- higher in energy

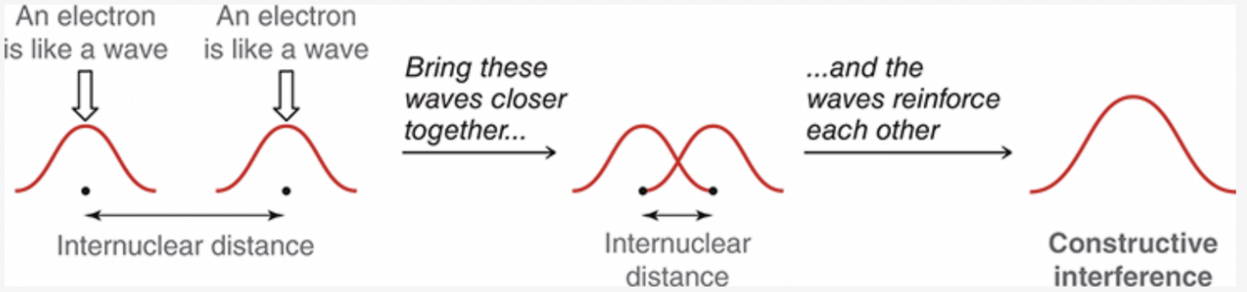
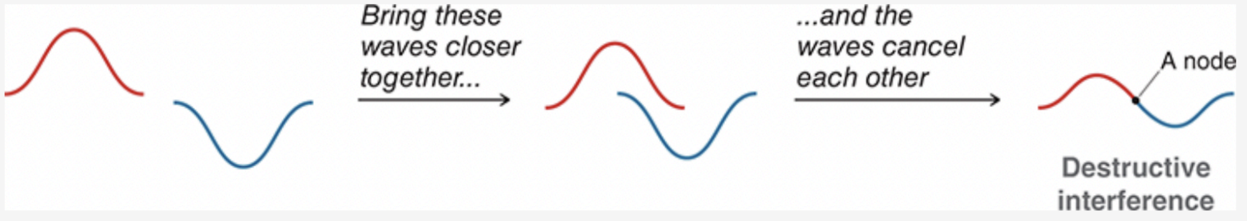


FIGURE 1.11 **Constructive interference resulting from the interaction of two electrons.**

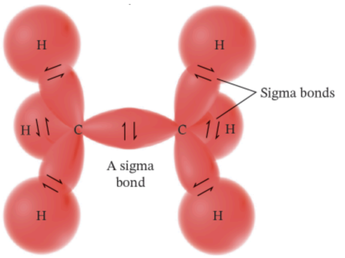
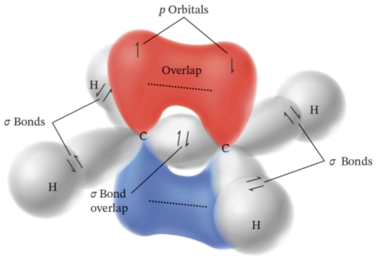
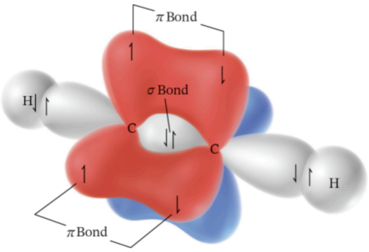
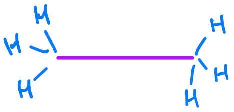
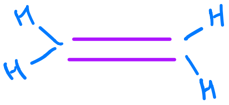
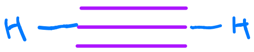


which molecular orbital will be formed first?

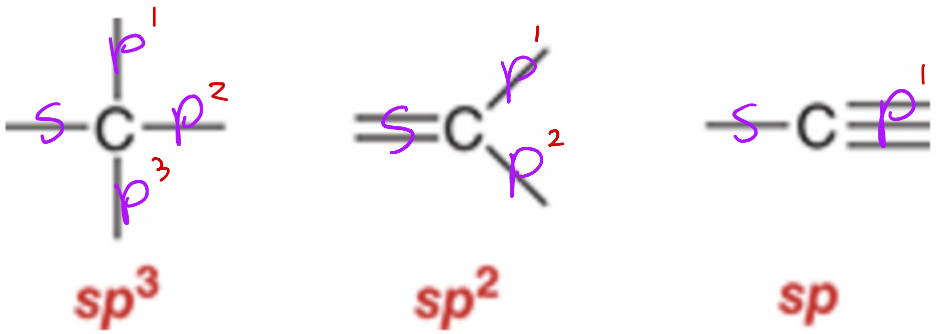
bonding MO

Hybridized Orbitals:

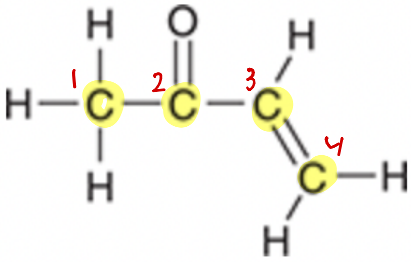
- A combination of pure atomic orbitals
- for this class we only focus on s and p

	Sp3	Sp2	Sp
Diagram			
What's Happening	A combination of 1s orbital and 3p orbitals	An overlap of p orbitals forms 1 pi bond	An overlap of p orbitals forms 2 pi bonds
Bond-line			
Geometry	tetrahedral	trigonal planar	linear
Angles	109.5°	120°	180°

Hybridization life hack!!!



Determine the hybridization state of each carbon:



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C1 = sp^3

C2 = sp^2

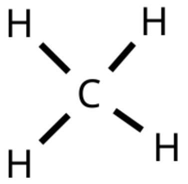
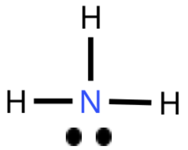
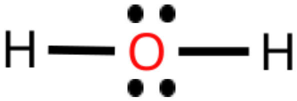
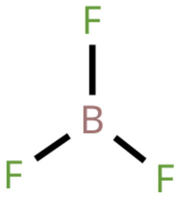
C3 = sp^2

C4 = sp^2

VSEPR Theory:

- valence Shell electron pair repulsion
- used to predict the geometry of an atom

Common Molecular Shapes:

Compound	Bonding e- pairs	Lone e- pairs	Steric number	Arrangement of e- pairs	Molecular Geometry
	4	0	4	tetrahedral	tetrahedral
	3	1	4	tetrahedral	trigonal pyramidal
	2	2	4	tetrahedral	Bent
	3	0	3	Trigonal planar	trigonal planar
H—Be—H	2	0	2	Linear	Linear

steric # = # single bond + # lone pairs

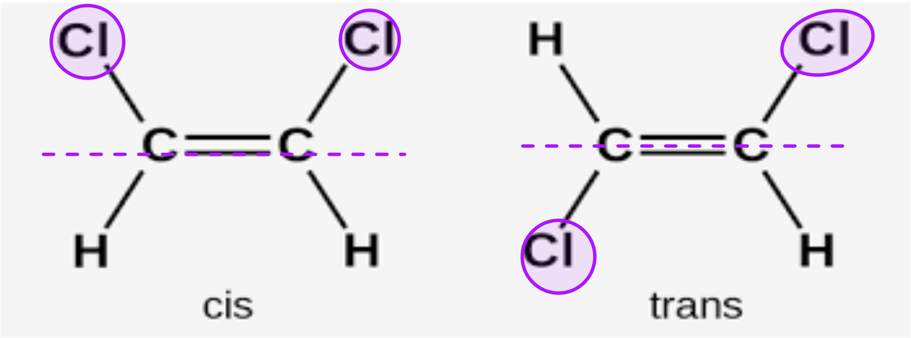
Cis/trans Steroisomerism:

Cis: on the same plane

Trans: on opposite ends of the plane

We can think of the molecule as being on a plane and separating this plane evenly either through the molecule itself or through a double/triple bond

Ex:



Restricted Rotation:

AKA, the properties of a single, double, and triple bond

Order the bonds:

Length

longest shortest

/ → // → ///

Energy

high low

/// → // → /

Strength

stronger weaker

/// → // → /