(5) **Today**

Sections 1.5-1.10
Valence Bond Theory

Sections 1.12
Drawing Chemical Structures

Next Class (6)

Sections 1.12
Drawing Chemical Structures

(7) **Second Class from Today**

Sections 2.1 - 2.4
Polar Covalent Bonds, Formal Charges,
Resonance/Electron Delocalization

Sections 2.4 – 2.6
Resonance/Electron Delocalization

Bring Modeling Kits to Class

Third Class from Today (8)

Sections 2.7 – 2.11
Acids and Bases

hybrid orbitals are used to form σ bonds and to hold lone-pair electrons

in the valence bond model, single bonds are always σ bonds

double and triple bonds are formed from σ bonds plus π bonds

# of σ bonds + pairs of lone-pair electrons = # of hybrid orbitals needed

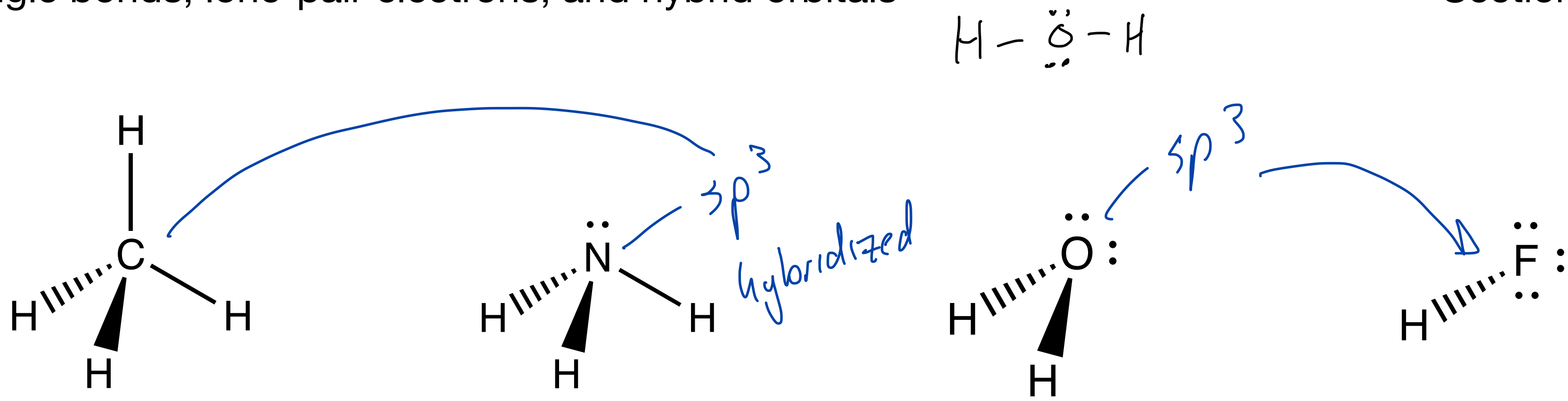
or

number of directions electrons must be pointed in = # of hybrid orbitals needed

VSEPR rules

count out the # of atomic orbitals need to make the hybrid orbitals
starting with the 2s orbital (or 3s if appropriate)

name the hybrid orbitals sp^n where n is the number of p orbitals used

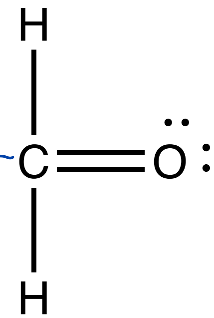


4 directions	4 directions	4 directions	4 directions
need 4 HO's	need 4 HO's	need 4 HO's	need 4 HO's
mix 4 AO	mix 4 AO	mix 4 AO	mix 4 AO
starting with	starting with	starting with	starting with
s × p × p × p	s × p × p × p	s × p × p × p	s × p × p × p
sp^3	sp^3	sp^3	sp^3

single bonds + lp e^-'s go in hybrid orbitals

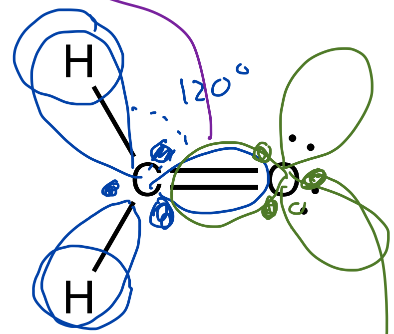
σ bonds

Identify atoms that use sp^3 hybrid orbitals to form bonds and hold lone-pair electrons sp2 hybrid on C overlaps with sp2 hybrid on O ... share e- make a bond



Apply VSEPR

rules



3 different directions (or 3 σ bonds)

3 HO's needed

2s + 2px + 2py

hybridize

sp2, sp2, sp2

parallel 2pz orbitals overlap, share e-'s, and form a π bond

3 different directions (or 1 σ bond + 2 sets lp e-'s)

3 HO's needed

2s + 2px + 2py

hybridize

sp2, sp2, sp2

2pz not hybridized

2pz not hybridized

https://www.westfield.ma.edu/cmasi/organic/hybrid/hybrid2.html

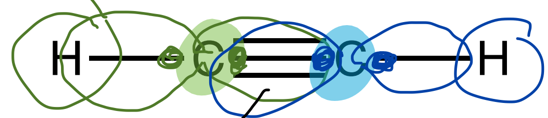
Identify atoms that use hybrid orbitals to form bonds and hold lone-pair electrons

double bonds are made σ bond + π bond

Triple bonds and sp? hybridization

Sections 1.5 - 1.10

the sp hybrid on C is overlapping with the 1s orbital on H … share e⁻'s … make a σ bond



C atom sets of e⁻'s point in 2 directions
2 HO's needed
2 AO's mixed
2s + 2p$_z$
⇓ hybridize
sp, sp

① sp hybrid is overlapping with sp hybrid … share e⁻'s … σ bond

C atom sets of e⁻'s point in 2 directions
2 HO's needed
2 AO's mixed
2s + 2p$_z$
⇓ hybridize
sp, sp

② 2p$_x$ is parallel to 2p$_x$
overlap… share e⁻'s …
make a π bond

③ 2p$_y$ is parallel to 2p$_y$
overlap… share e⁻'s …
make a π bond

https://www.westfield.ma.edu/PersonalPages/cmasi/organic/hybrid/hybrid2.html

Identify atoms that use hybrid orbitals to form bonds and hold lone-pair electrons

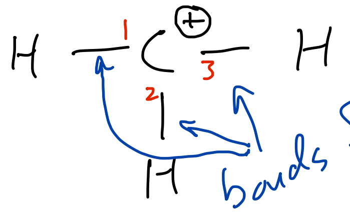
triple bond = 1σ + 2π

The methyl cation, anion, and radical

carbocation

$FC_z = 4 - (3) = +1$

CH_3^+ ← empty orbital... unhybridized 2pz



bonds formed from sp^2 hybrids overlapping with 1s orbitals on H's

C 4 ve⁻

3H 3(1) ve⁻

− 1e⁻ ⊕ charge

6 e⁻ 3 pairs

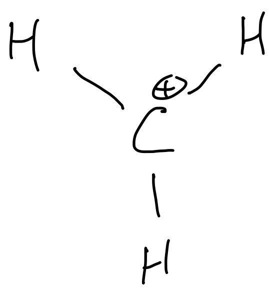
3 directions

3 HO's needed

3 AO's mixed

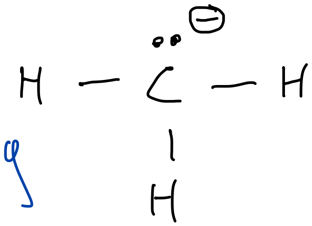
2s, 2px, 2py

⇓



sp^2, sp^2, sp^2

CH_3^-



4 directions

4 HO

4 AO's mixed

2s, 2px, 2py, 2pz

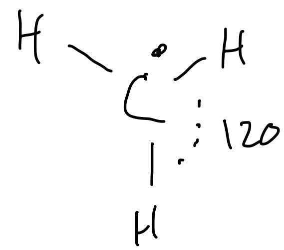
⇓ hybridize

sp^3, sp^3, sp^3, sp^3

"radical" means odd # of e⁻'s

$CH_3^\bullet$

⇓

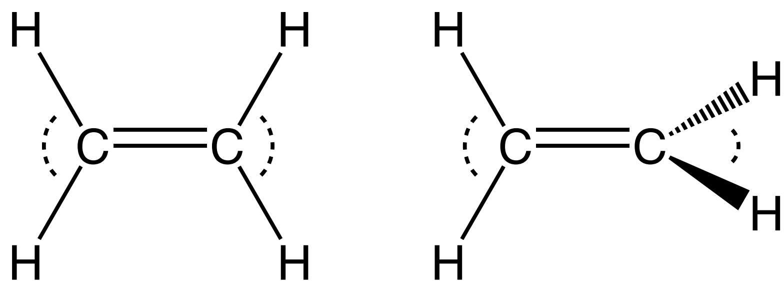


3 directions

sp^2

Determine the hybridization of unusual molecular fragments

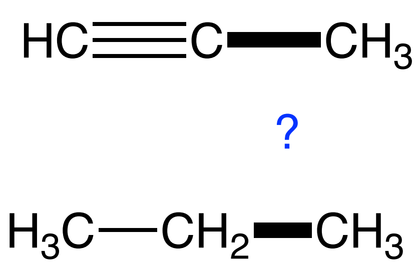
What can we use Valance Bond Theory for?



Which one? Both C atoms are trigonal planar

Why is there free rotation around C to C single bonds but not C to C double bonds?

Which bond is stronger?



Explain observations and make predictions based on the hybridization of an atom

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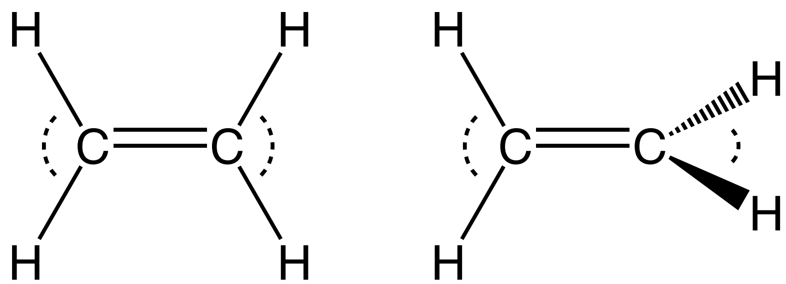

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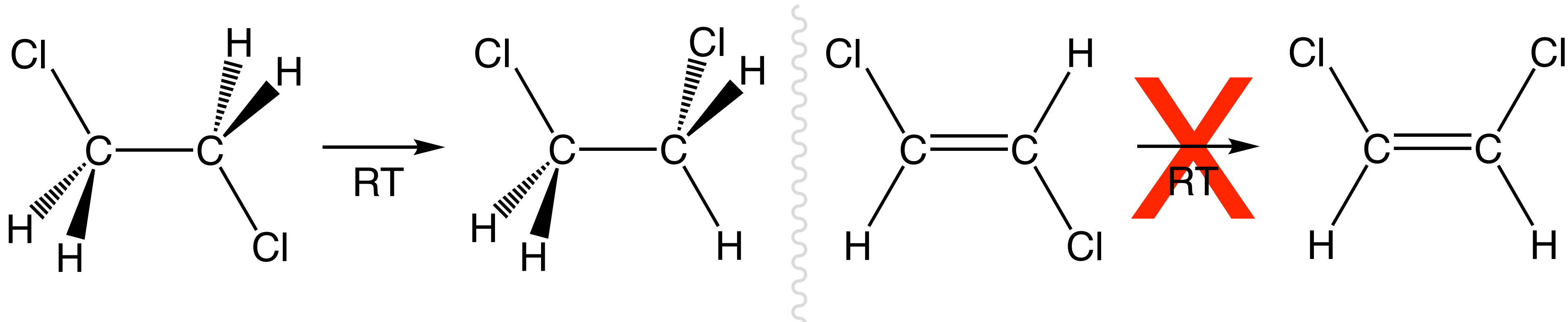

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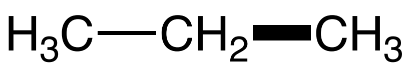
What can we use Valance Bond Theory for?

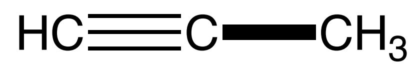
Which bond is strongest?

370 kJ/mol[2], 355±8 kJ/mol[3]



426 kJ/mol[1]

490 kJ/mol[4]



[2] Organic Chemistry, 10th ed. McMurry.

[3] Chem. Rev. **66**, 465 (1966).

[4] J.Chem.Ed. **42**, 502 (1965)

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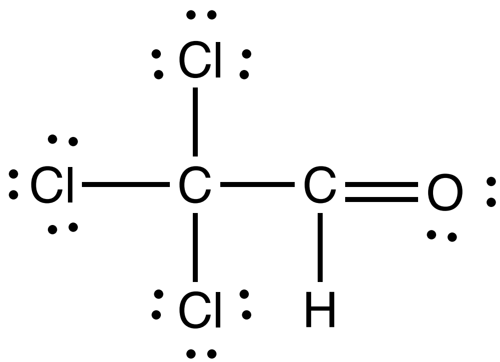
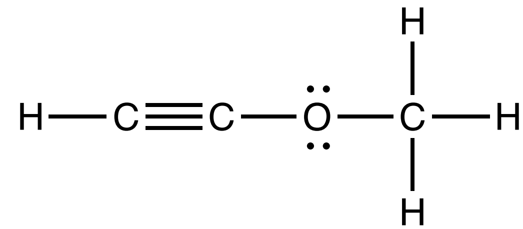
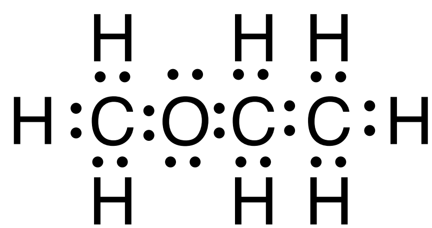
Practice





$$N\equiv C-CH_2-NH_2$$



Chemists use different drawings to place emphasis on different aspects of a molecule.

Representations are used to solve typographical issues.

Molecular Formulas as Compared to Condensed Structures/Structural Formulas

In organic, molecular formulas are written C_xH_y(and other elements listed alphabetically)

C_3H_8O

In organic, condensed structures typically start with a C, and everything immediately to the right of the C is connected to that first C. When the the first C is finally connected to the second C, now that atoms right of the second C are connected to second C. In acyclic unbranched molecules atoms to the right of the second C are not connected to the first C.

C_3H_8O $CH_3CH_2OCH_3$ $CH_3CH_2CH_2OH$ $CH_3CHOHCH_3$

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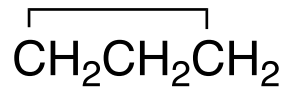
CH_2CHCH_3

Because bonds are not drawn, condensed structures require the reader to bring some chemical knowledge to their interpretation.

Condensed Structures/Structural Formulas: Cyclic Molecules



Condensed Structures/Structural Formulas: Using ( )

$CH_3CH(OH)CH_2CH_3$ $CH_3(CH_2)_3CH_3$ $CH_3CH_2CH(CH_3)_2$

Parentheses **( )** in structures are typically used to set off side chains, to indicate a repeating unit, or to indicate multiple groups of the same structure.

Often, chemists omit parentheses when they are not absolutely necessary,

$CH_3(CH_2)_3CH_3$

$CH_3CHOHCH_3$

$CH_3CH(OH)CH_3$

$CH_3COCH_2CH_3$

$CH_3C(O)CH_2CH_3$

and sometimes chemists do things for aesthetic reasons.

$C(CH_3)_3OH$ $CH_3C(CH_3)_2OH$ $(CH_3)_3COH$

Convert Condensed Structures to Kekulé Structures

$CH_3CHOHCH_2CH_3$

$CH_3C(O)CH(CH_3)_2$

CH_3CHO

When a bond ends and the atom isn't labeled it is assumed to be C.

When there aren't enough bonds drawn to a C atom, the “missing” bonds are C atom to H atom bonds.

All other atoms are labeled.

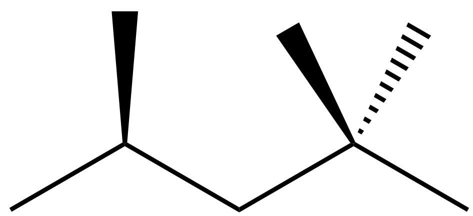
Heptane

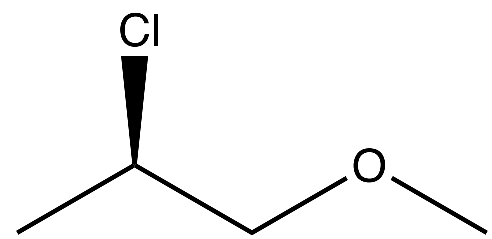
2-heptanol

Different structures serve different purposes, but they represent the same things

Converting Between Structure Types

Sections 1.12





$CH_3CH(OH)CH_2CH(CH_3)CH_2CH_3$