(3) **Today**

Sections 1.5-1.10
Valence Bond Theory

Skipping Section 1.11 for now
An introduction to Molecular Orbital Theory

Sections 1.12
Drawing Chemical Structures

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

Next Class (4)

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

Sections 2.4 – 2.6
Resonance/Electron Delocalization

(5) **Second Class from Today**

Sections 2.4 – 2.6
Resonance/Electron Delocalization

Sections 2.7 – 2.11
Acids and Bases

Third Class from Today (6)

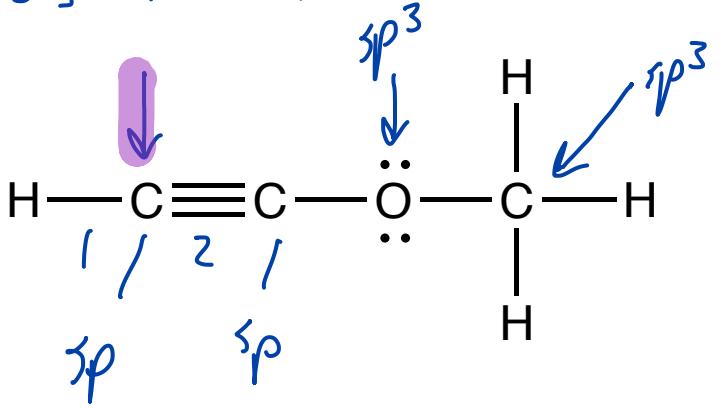
Sections 2.7 – 2.11
Acids and Bases

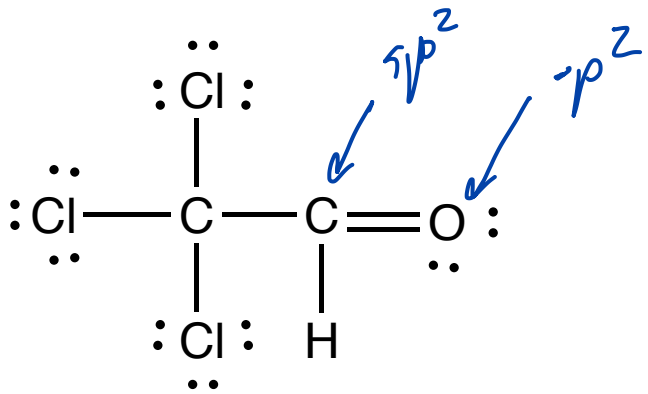
Practice: Determine the Hybridization of the Atoms in the Following Molecules

# of HO's Needed can also use # of groups of e⁻'s to determine # HO's
σ bonds + # pairs of lone-pair e⁻'s

count out # of AO's needed
2s x 2p x etc

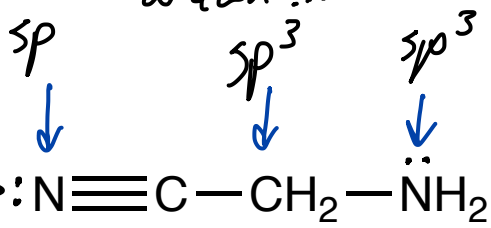
name the hybrids
sp^3 made from one s and **three** p orbitals
sp^2 made from one s and **two** p orbitals
sp made from one s and **one** p orbital





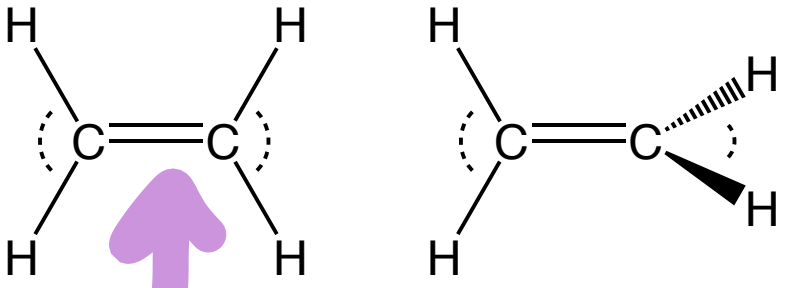
C to H σ bonds not drawn ...

lone-pair e⁻'s are not drawn but they are there because we understand that this N has a complete octet of e⁻'s



condensed structure

What can we use Valance Bond Theory for?

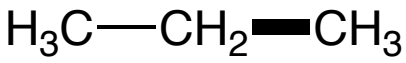


Which one? Both C atoms are trigonal planar

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

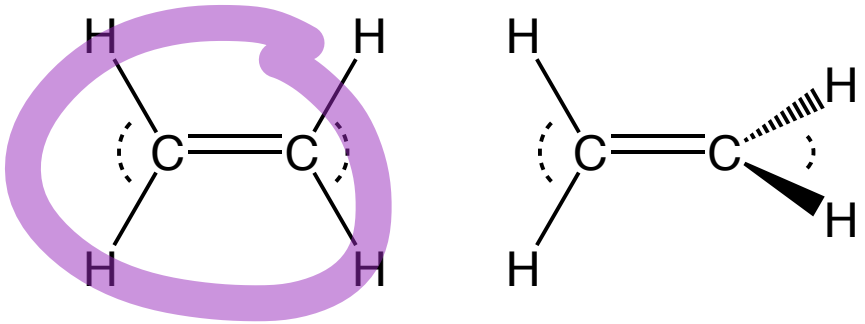
Which bond is stronger?

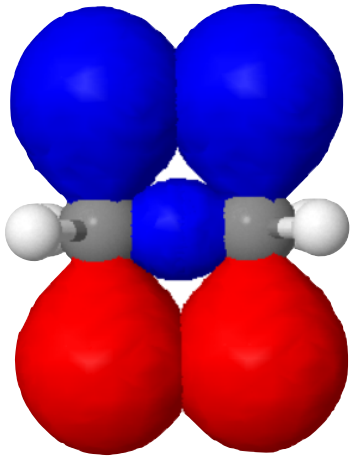
?



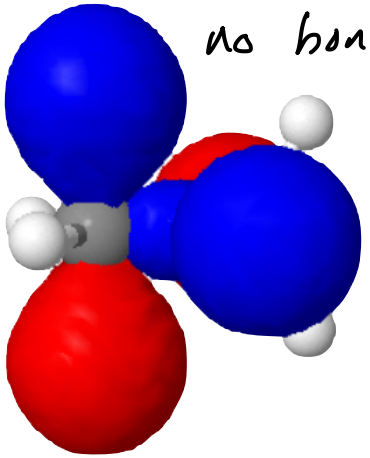
Explain observations and make predictions based on the hybridization of an atom

What can we use Valance Bond Theory for?





no overlap, no bond



Which one? Both C atoms are trigonal planar

To form the π bond unhybridized p orbitals on each C atom need to be parallel to each other.

Since all the p orbitals are perpendicular to each other, to get two unhybridized orbitals that are parallel, the p orbitals that use to make the hybrids need to be coplanar. For π bond to form from two paralled $2p_x$ orbitals the hybrids would have to be made From $2p_y$ & $2p_z$ orbitals

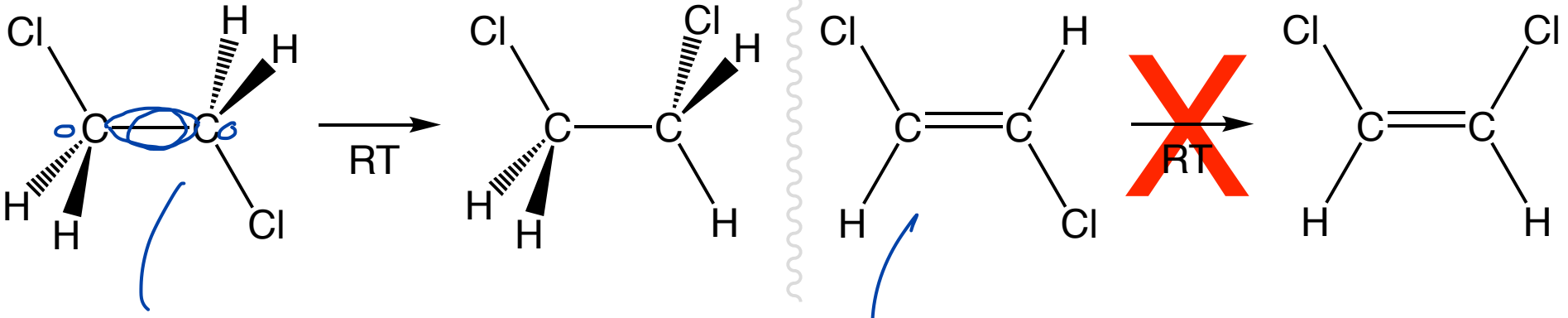
Explain observations and make predictions based on the hybridization of an atom

What can we use Valance Bond Theory for?

sp^x $x+y=$ # HB's

sp^3

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



rotation around C-C bond doesn't change the orientation of the sp^3 hybrids forming the C to C bond so rotation can occur

rotation would require changing the orientation of the unhybridized p orbitals, which means they wouldn't be parallel, they would no longer overlap and the bond would break

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

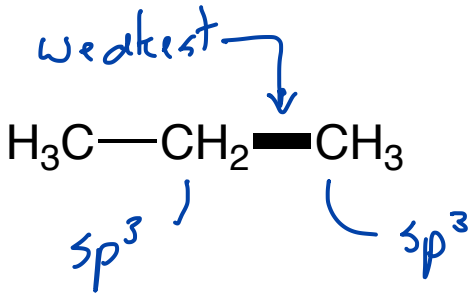
What can we use Valance Bond Theory for?

sp^2 — 1 parts s / 3 parts total

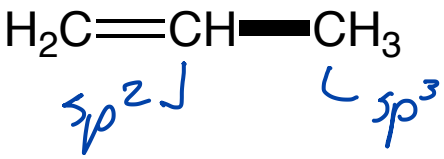
mix 1 part s with 2 parts p

Which bond is strongest?

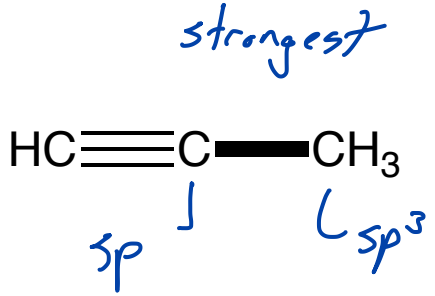
370 kJ/mol[2], 355±8 kJ/mol[3] — 426 kJ/mol[1] — 490 kJ/mol[4]



25% s 75% p



33% s + 67% p



hybrids are

50% s + 50% p

character character

s orbitals get e⁻'s closer to the nucleus

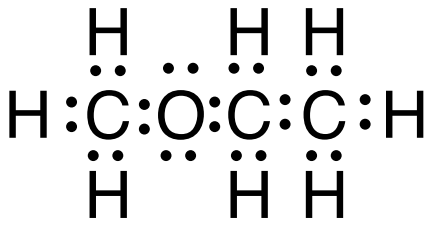
e⁻'s in s orbitals are lower in E

as s character increases e⁻'s get closer to the nucleus, and lower in E. The bond made from hybrids with the highest s character will have the lowest E e⁻'s and be the strongest.

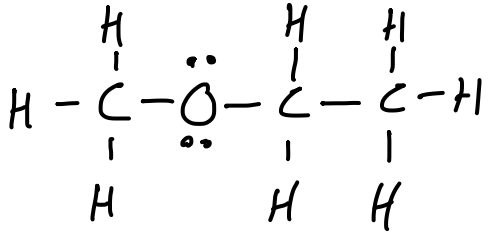
[2] Organic Chemistry, 10th ed. McMurry.

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

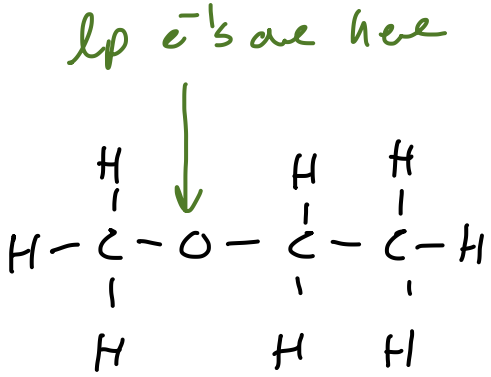
[4] J.Chem.Ed. **42**, 502 (1965)



Lewis Dot



Kekulé or line-bond



Kekulé structure
lone-pair e⁻'s are understood

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

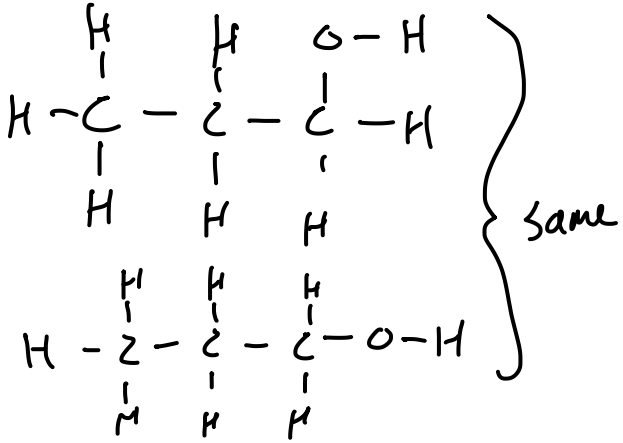
Representations are used to solve typographical issues.

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

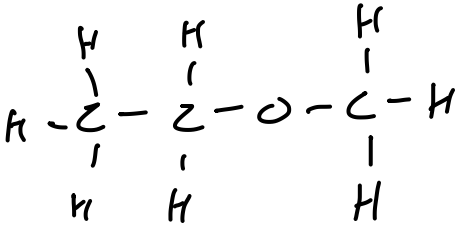
C_3H_8O C_3H_7ClO

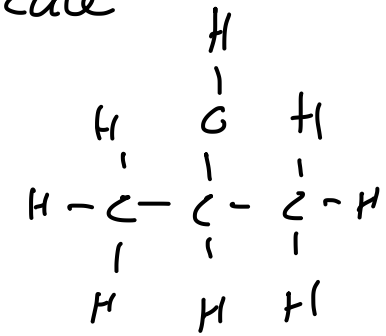
not specific enough to represent only 1 molecule

this gives us no information about the structure only the number of atoms in the molecule



same

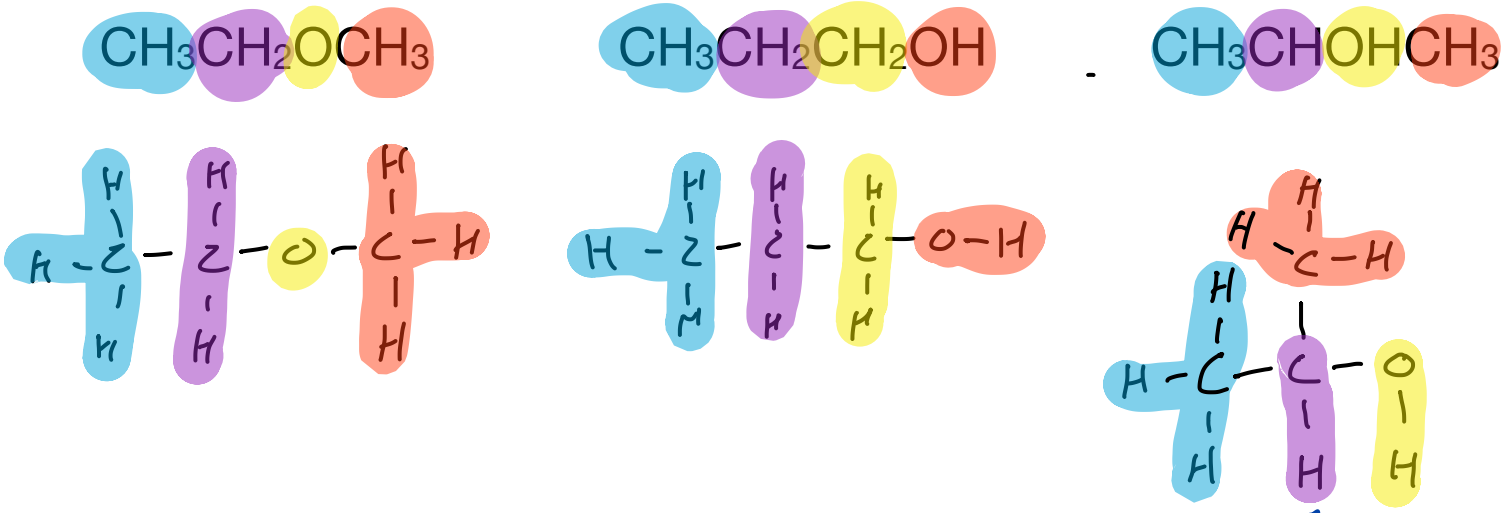




structural (constitutional) isomer

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

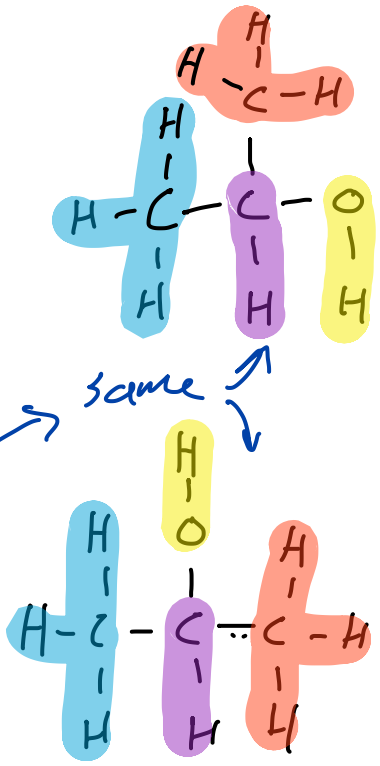


C

typical # of bonds

4	3	2	1	0
C	N	O	F	Ne

since OH is bonded to the middle C atom in both of these drawings, these are just different drawings of the same molecule



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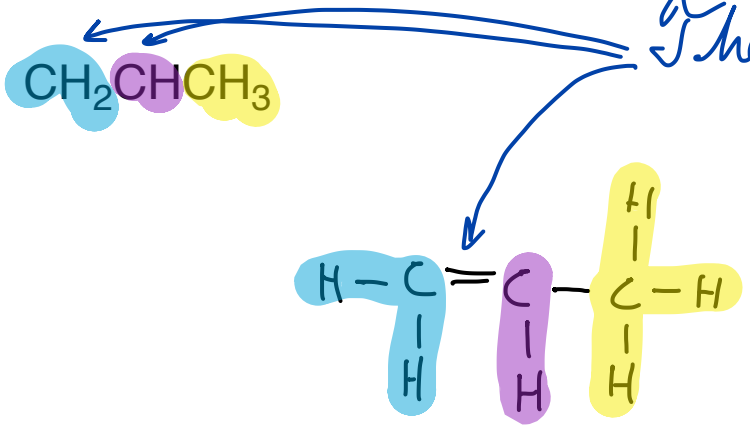


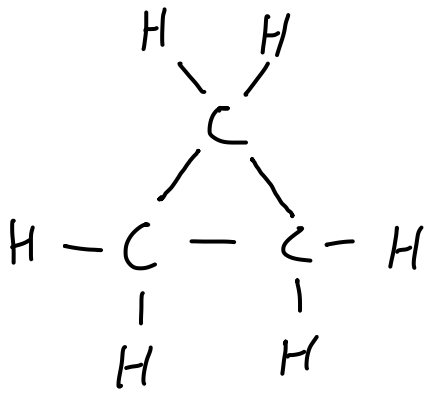
There are no charges on these C atoms so we must assume that they are forming the 4 expected bonds.

The only way to get both C atoms to 4 bonds is to have a double bond

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

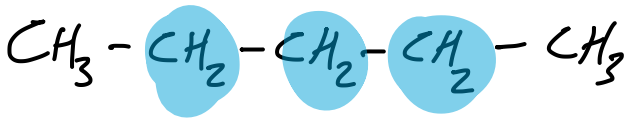
$CH_2CH_2CH_2$

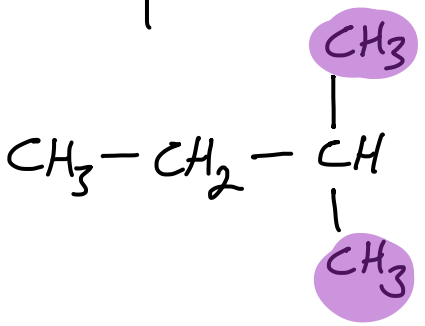
a simplified way to say C_1 is bonded to C_3



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

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,

$CH_3(CH_2)_3CH_3$

makes no sense without parentheses

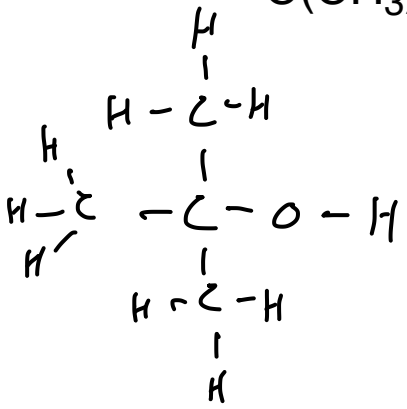
$CH_3CHOHCH_3$ $CH_3CH(OH)CH_3$

you'll have to recognize this is a branch, that the H after to O is bonded to the O, based on chemical knowlege

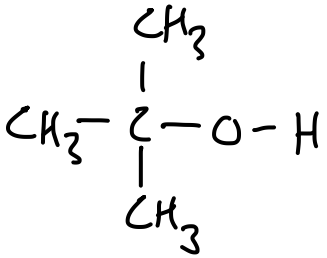
$CH_3COCH_2CH_3$ $CH_3C(O)CH_2CH_3$

and sometimes chemists do things for aesthetic reasons.

$C(CH_3)_3OH$

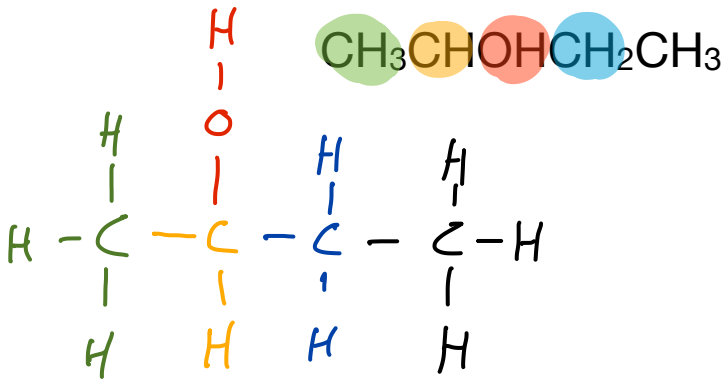


$CH_3C(CH_3)_2OH$

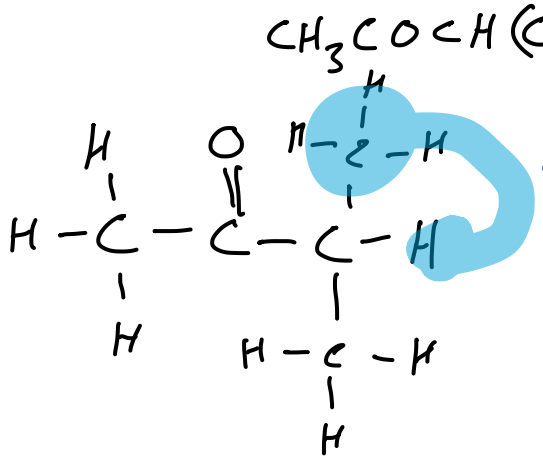


$(CH_3)_3COH$

done to emphasize connection between C + O



$CH_3C(O)CH(CH_3)_2$



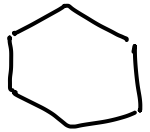
CH_3 group can be in either position and the drawing would represent the same molecule

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

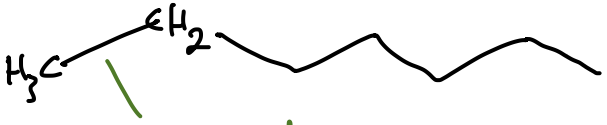
When there aren't enough bonds drawn to a C atom, the "missing" bonds are C atom to H atom bonds.

All other atoms are labeled.

C_6H_{12}

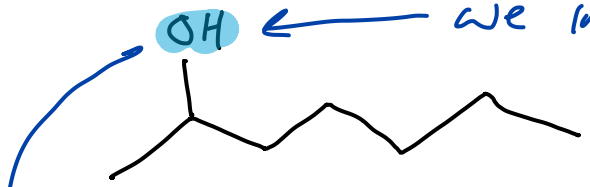


Heptane $CH_3CH_2CH_2CH_2CH_2CH_2CH_3$

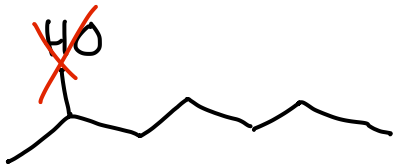


1 bond drawn ... no charges so normal bonding is occuring need 3 more bonds to get to 4 so those bonds are assumed to be to H atoms

2-heptanol $CH_3CHOH(CH_2)_4CH_3$



← we include the H

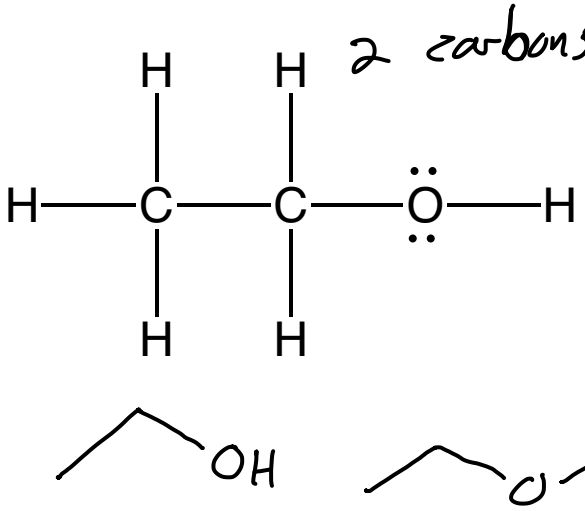


draw the non C atom next to the bond

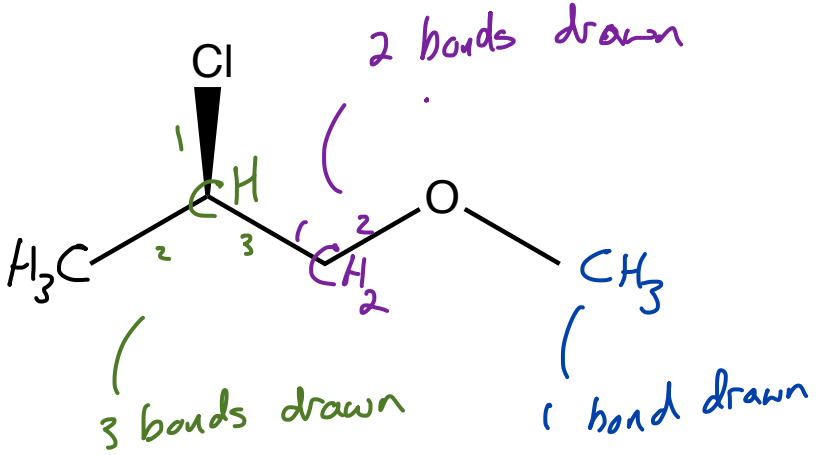
Different structures serve different purposes, but they represent the same things

$CH_3CH_2CH_2CH_3$

convert Lewis to skeletal

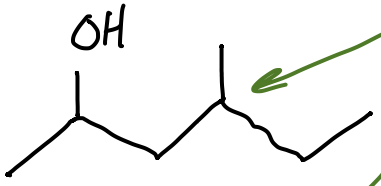


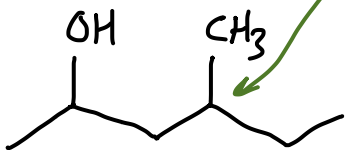
convert skeletal to condensed



convert structural formula to skeletal

$^{1}CH_3\,^{2}CH(OH)\,^{3}CH_2\,^{4}CH(CH_3)\,^{5}CH_2\,^{6}CH_3$





all in plane?
I thought that wasn't possible

Correct! So when only straight lines are used it means no attempt is being made to show the shape or stereochemistry of the molecule

convert skeletal to condensed