(6) **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

Next Class (7)

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

Sections 2.4 – 2.6
Resonance/Electron Delocalization

(8) **Second Class from Today**

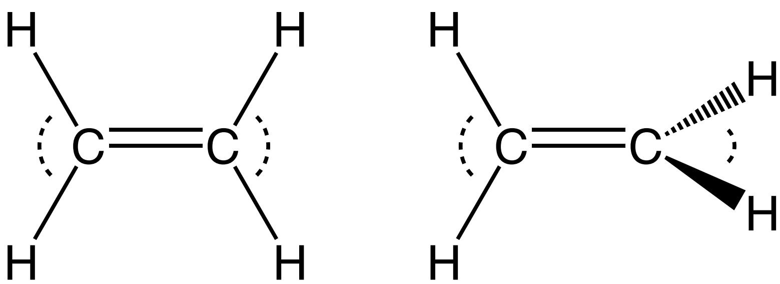
Sections 2.4 – 2.6
Resonance/Electron Delocalization

Sections 2.7 – 2.11
Acids and Bases

Third Class from Today (9)

Sections 2.7 – 2.11
Acids and Bases

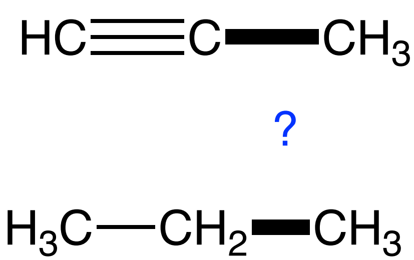
What can we use Valance Bond Theory for?



Which one? Both C atoms are trigonal planar

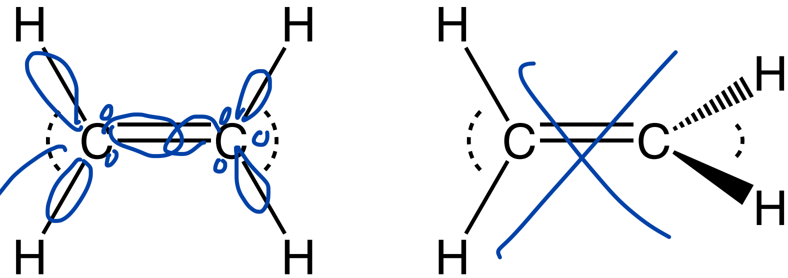
Why is there free rotation around C to C single bonds but not C to C double bonds?

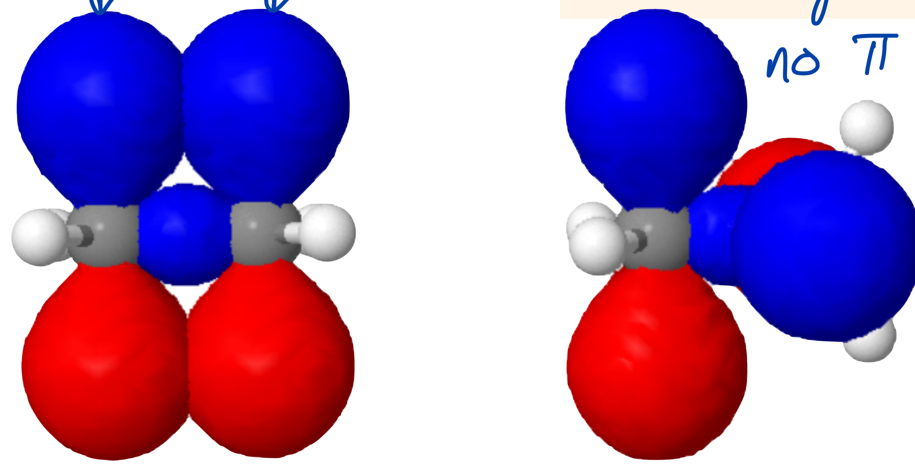
Which bond is stronger?



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

What can we use Valance Bond Theory for?





Which one? Both C atoms are trigonal planar

sp² hybridized … 3 directions … 3 HO's needed… 2s, 2px, 2py ⇒ sp², sp², sp²
3 σ bonds

the 1st bond in the double bond is made from overlapping sp² hybrids

the 2nd bond is made from parallel overlapping 2pz orbitals + they form the π bond

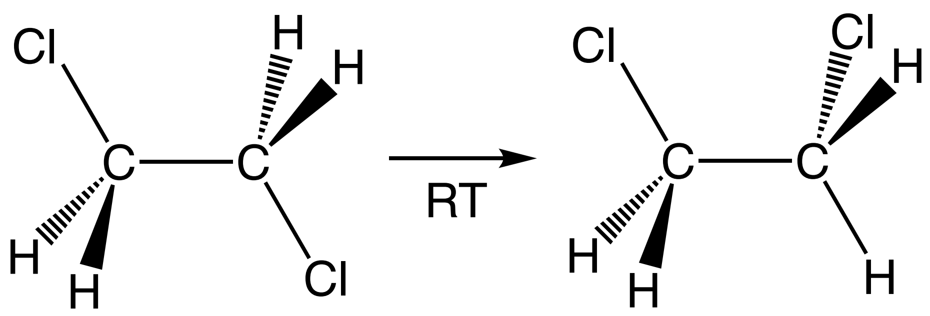
since the hybrids made from 2px + 2py are ⊥ to the 2pz all hybrids must be in the same plane so 2pz orbitals overlap

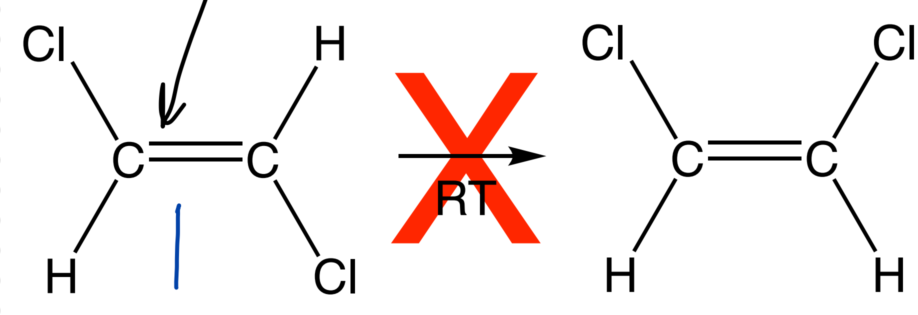
Explain observations and make predictions based on the hybridization of an atom

What can we use Valance Bond Theory for?

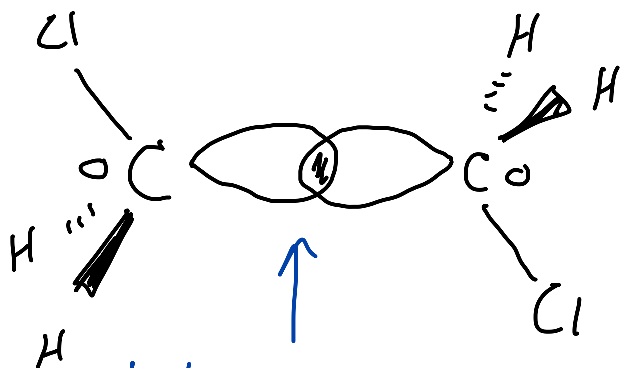
you have to break the π bond to do the rotation

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

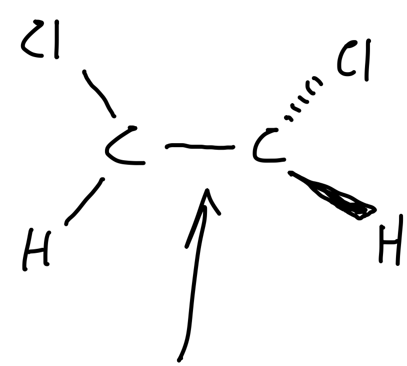




π bond made from 2p orbitals ⊥ to σ bonds



rotation doesn't cause a change in the orientation of the hybrid... so free rotation is possible

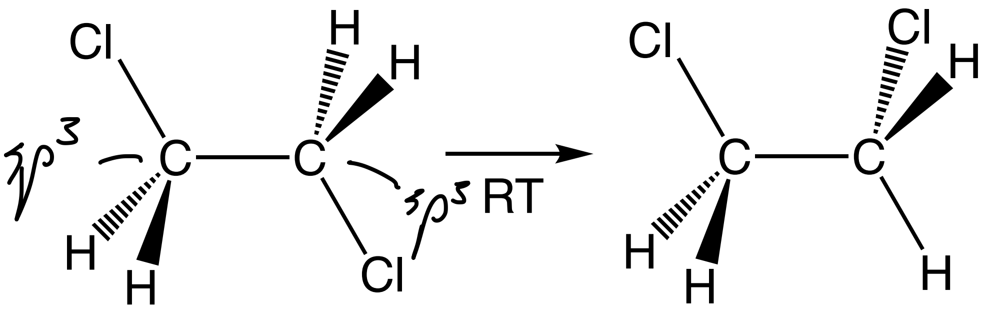


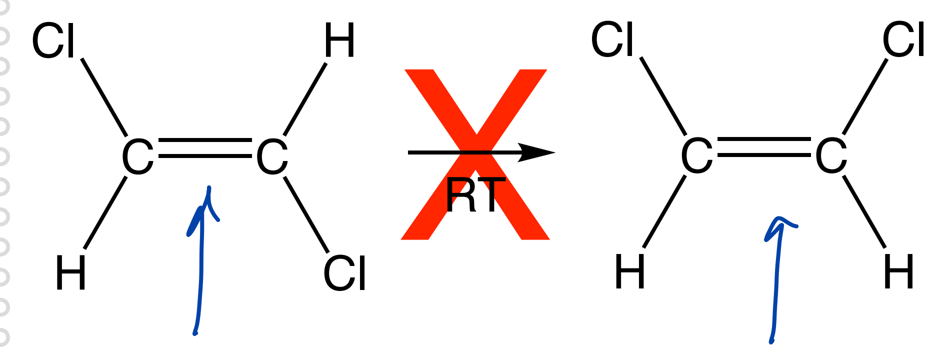
db is lost during rotation

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

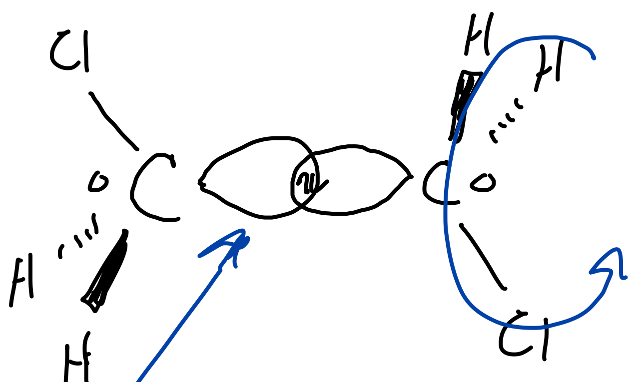
What can we use Valance Bond Theory for?

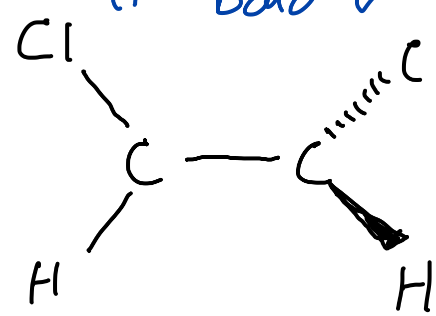
Why is there free rotation around C to C single bonds but not C to C double bonds?





coplanar σ bonds... ∥ p orbitals
π bond ✓





rotation along the bond does not change the orientation of the orbitals

rotation caused the p orbitals to be ⊥ ... which means the π bond has to be broken to rotate

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

What can we use Valance Bond Theory for?

Which bond is strongest?

$H_3C-CH_2-CH_3$	$H_2C=CH-CH_3$	$HC\equiv C-CH_3$
370 kJ/mol[2], 355±8 kJ/mol[3]	426 kJ/mol[1]	490 kJ/mol[4]

weaker σ bond

sp^3 sp^3

CH_2 is

25% s + 75% p

sp^2 sp^3

33% s + 67% p

stronger σ bond

sp sp^3

50% s + 50% p

looks more like → 50% s character

s . . .

gets e^-'s close to the nucleus . . . e^-'s are lower in E

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

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

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

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370 kJ/mol[2], 355±8 kJ/mol[3]	426 kJ/mol[1]	490 kJ/mol[4]
weakest C–C bond		strongest C–C bond
sp^3 — sp^3	sp^2 — sp^3	sp — sp^3
1 part s 3 parts p	1 parts 2 parts p	1 part s 1 part p
25% s 75% p	33% s 67% p	50% s 50% p

s character increases from sp^3 to sp

s orbitals get e^-'s closer to nucleus

the higher the s character the more the e^-'s can be close to the nucleus

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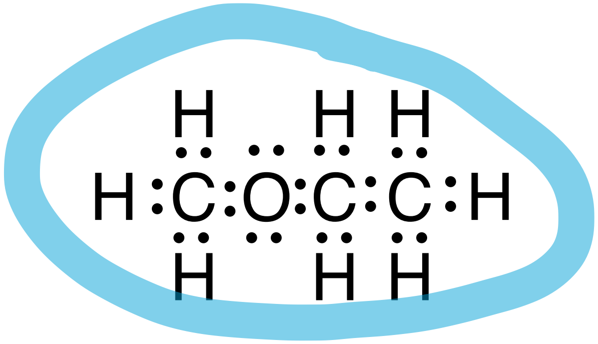
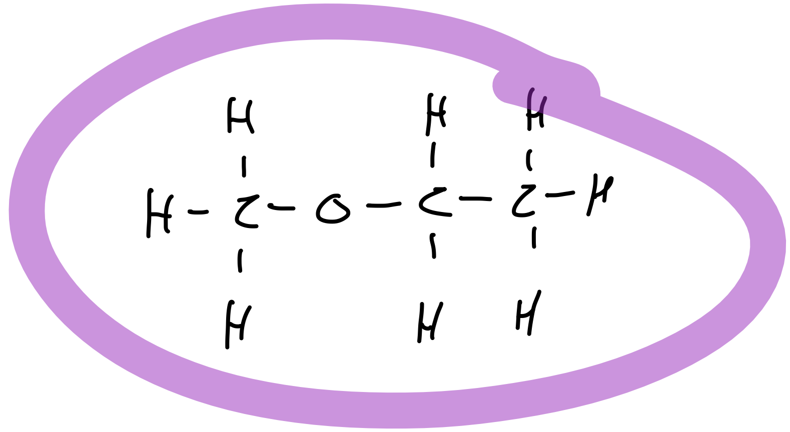
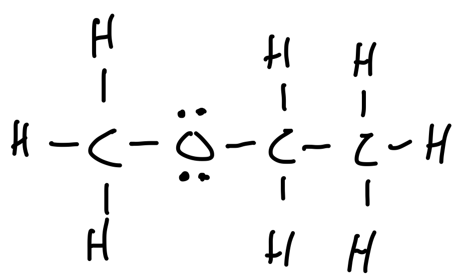
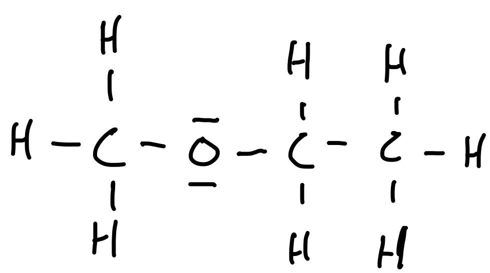
Representing Molecules: Lewis & Kekulé Structures







Kekulé structures leave out lp e^-'s even though they are there



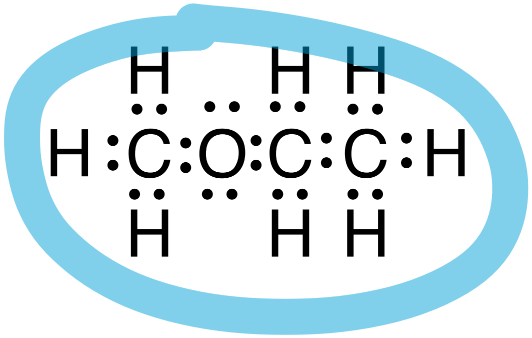
We must still follow the octet rule, so even though we've only drawn 4 on O the other 4 are understood to be there

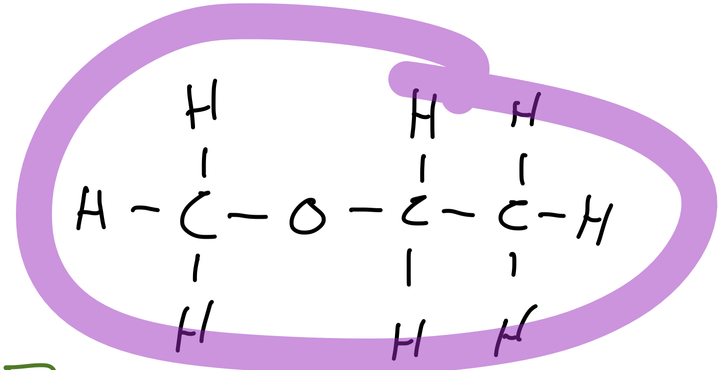
Chemists use different drawings to place emphasis on different aspects of a molecule.

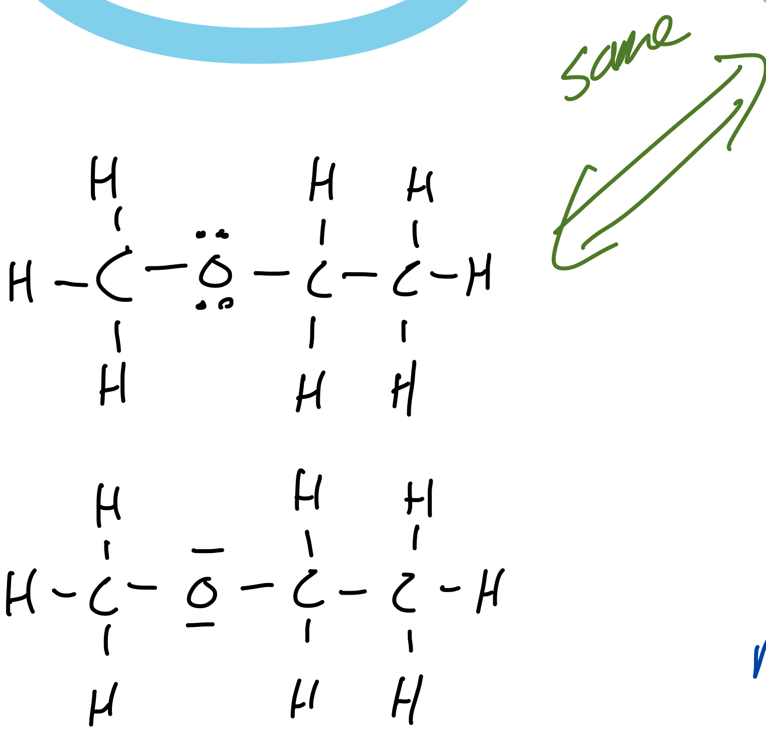
Representations are used to solve typographical issues.

Representing Molecules: Lewis & Kekulé Structures

Section 1.12







The octet rule is still followed so even though we haven't drawn the 2 pairs of lp e⁻'s they are there.

No charge is indicated which means we have the expected # of e⁻'s so...

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)

For example:

$12e^- + 8e^- + 6e^-$

$26e^-$

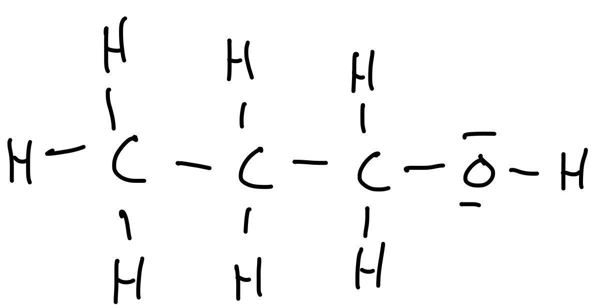
13 pairs

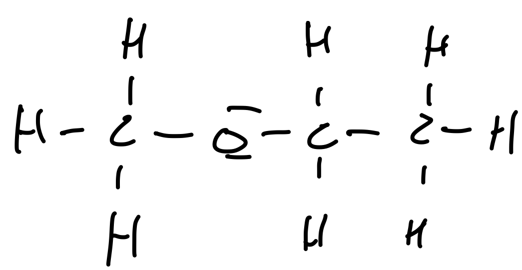
C_3H_8O C_3H_7ClO

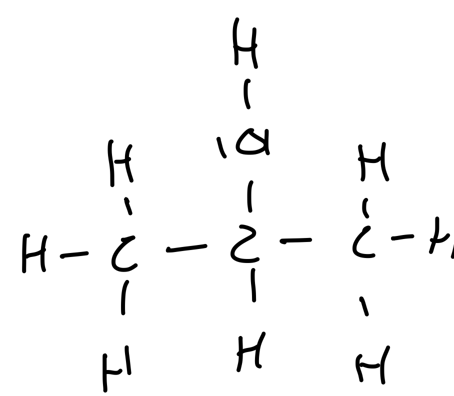
C's are good as middle atoms because they make 4 bonds

H's go around the edges because they make 1 bond

O's can go inbetween because they make 2 bonds







leave out bonds + lp e^-'s

$CH_3CH_2CH_2OH$

$CH_3OCH_2CH_3$

$CH_3CH(OH)CH_3$

$CH_3CHOHCH_3$

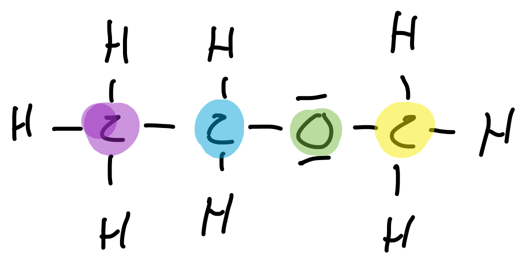
Molecular Formulas as Compared to Condensed Structures/Structural Formulas

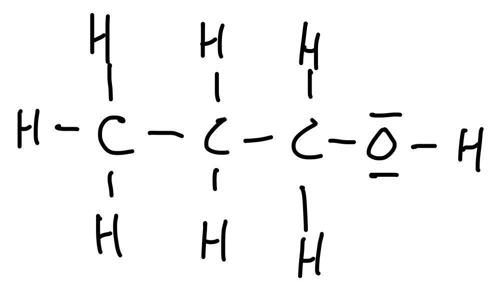
Section 1.12

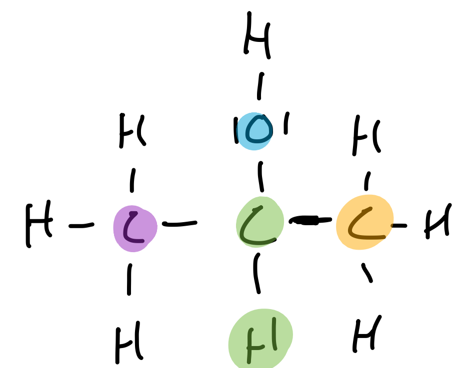
Bonds + lp e^{-}'s are omitted

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 $CH_3CH_2OCH_3$ $CH_3CH_2CH_2OH$ $CH_3CH(OH)CH_3$







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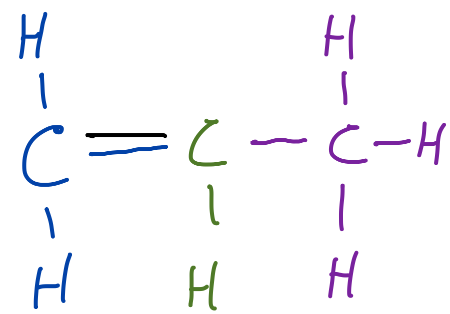
CH_2CHCH_3

Kekulé structure



C bonded to 2 H's
then
C bonded to 1 H
C bonded to 3 H's

$18e^-$ ✓

$3 * 4 = 12e^-$

$6 * 1 = 6e^-$

$18e$ ✓

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

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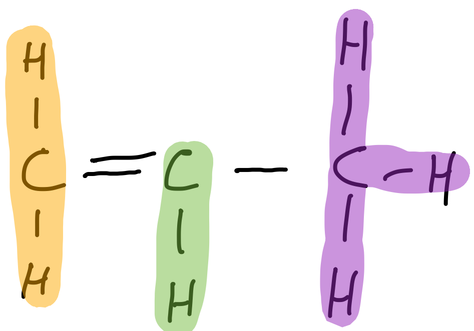
CH_2CHCH_3

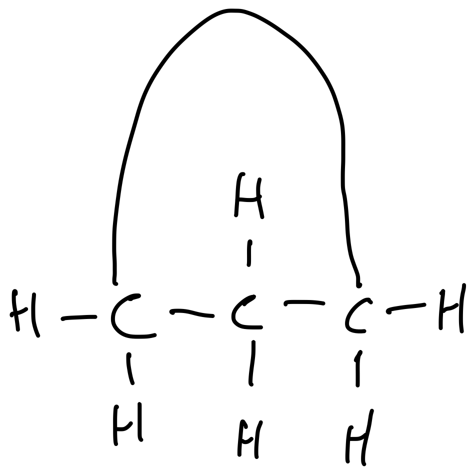


$3 \cdot 4 = 12\ e^-$

$6 \cdot 1 = 6\ e^-$

$18\ e^-$ 9 pairs

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



$CH_2CH_2CH_2$ rings/cyclic molecules

1st C is bonded to 3rd C

bracket shows that a ring has formed