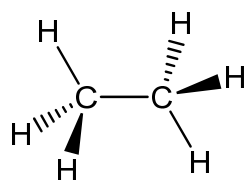


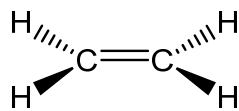
Chapter 2 – Hybridization, 2D and 3D Structures – These are the three shapes we have to explain

ethane

tetrahedral carbon atoms
 sp^3

HCH bond angles $\approx 109^\circ$

HCC bond angles $\approx 109^\circ$



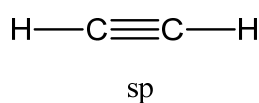
ethene

trigonal planar carbon atoms

sp^2

HCH bond angles $\approx 120^\circ$ (116°)

CCH bond angles $\approx 120^\circ$ (122°)

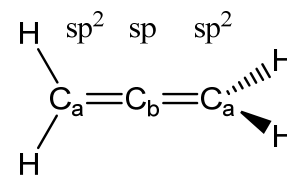


ethyne

linear carbon atoms

sp

HCC bond angles = 180°



allene

trigonal planar carbon atoms
at the ends and a linear
carbon atom in the middle

HC_aH bond angles $\approx 120^\circ$

HC_aC_b bond angles $\approx 120^\circ$

$C_aC_bC_a$ bond angles = 180°

Hybridization is how we are going to explain it (the shapes above).

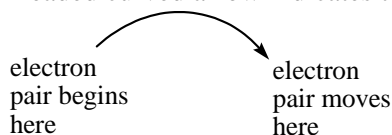
Concise Rules for Drawing 2D Lewis Structures, including resonance structures

1. Draw a sigma skeletal framework showing all of the sigma bonds from the condensed line formula.
2. Sum all of the valence electrons available for bonding and lone pairs. Reduce this number by 1 for each positive charge and increase this number by 1 for each negative charge.
3. Each sigma bond counts for two electrons. Subtract this number of electrons from the total number of electrons to determine how many electrons are available for lone pairs and pi bonds.
4. Use any remaining electrons as lone pairs to fill in octets on electronegative atoms first ($F > O > N > \text{other halogens} > C$). If the electrons are still not used up, add the additional electrons to carbon atoms at alternate positions to maximize charge separation where possible (minimize electron-electron repulsion) until all electrons have been used. It is helpful for you to write in the formal charge at this point (but not necessary). Formal charge will suggest the best way to group lone pair electrons used to make pi bonds.
5. A lone pair of electrons on an atom next to a neighbor with an incomplete octet can be shared to form a second (double) or third (triple) bond with the neighbor atom (these will be pi bonds). If this can be done to a particular electron deficient atom by more than one neighbor atom, then resonance structures are present. The best resonance structure will have the maximum number of bonds. If two structures have the same number of bonds, then a secondary consideration is to minimize charge separation (the formal charge from rule 4 will help here). If residual charge is necessary, it is better to be consistent with electronegativity (e.g. negative formal charge is better on oxygen than on carbon). Your goals, in this order, are 1. to maximize the number of bonds and 2. to minimize formal charge and 3. to keep formal charge consistent with electronegativity, if the other two goals have been met.
6. Resonance structures require a specific use of arrows.
 - a. Double headed arrows are placed between resonance structures.



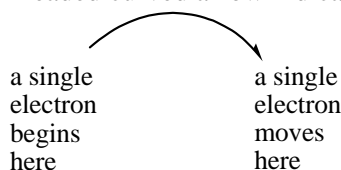
A double headed resonance arrow shows that these structures both contribute to an actual structure that cannot be drawn as a simple single Lewis structure.

b. A full headed curved arrow indicates two electron movement.



A full headed curved arrow indicates two electron movement to show where an electron pair will be located in the "next" structure, whether used in resonance structures or used in a reaction equation.

c. A half headed curved arrow indicates one electron movement.



A half headed curved arrow indicates one electron movement to show where an electron will be located in the "next" structure (as in free radicals), whether used in resonance structures or used in a reaction equation.

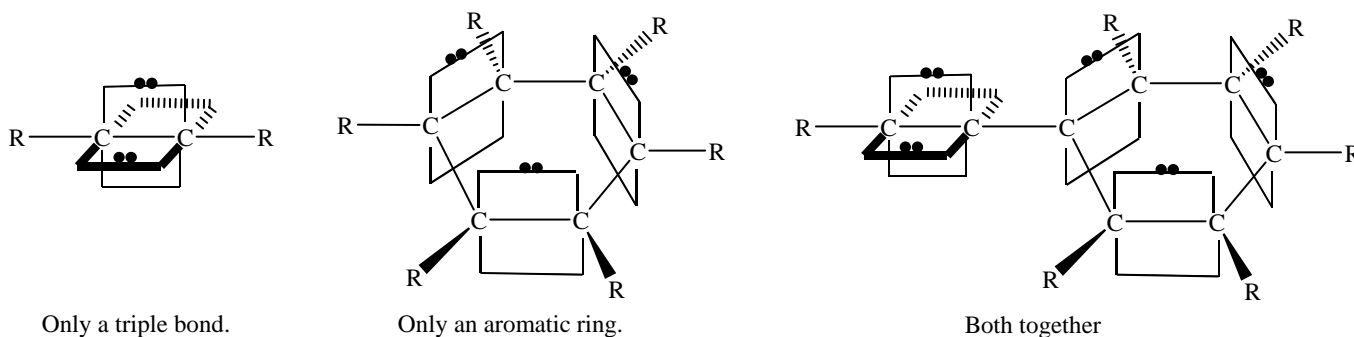
Guidelines for Three Dimensional Lewis Structures – build molecular models to visualize the structures

Guideline 1 – Draw a 2D Lewis structure as described above. This will allow you to determine the connections of the atoms, the hybridization, the shape, the bond angles, the number of sigma and pi bonds and the nature of any lone pairs of electrons.

Guideline 2 – Draw all reasonable 2D resonance structures to allow a determination of each atom's hybridization. We mentioned this idea several times in the 2D examples above, but we will explicitly state it again. The hybridization of any atom is determined by the resonance structure in which that atom has its maximum number of bonds. This is a very important idea that you will probably overlook on occasion. If I make a big deal about it here, maybe you won't forget about it...but you probably will!

Guideline 3 – Place as many atoms as possible in the plane of the paper when you begin to draw your 3D structure. You only need to know how to draw three different shapes (sp , sp^2 and sp^3), but you really need to know how to draw them well.

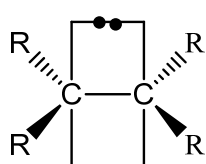
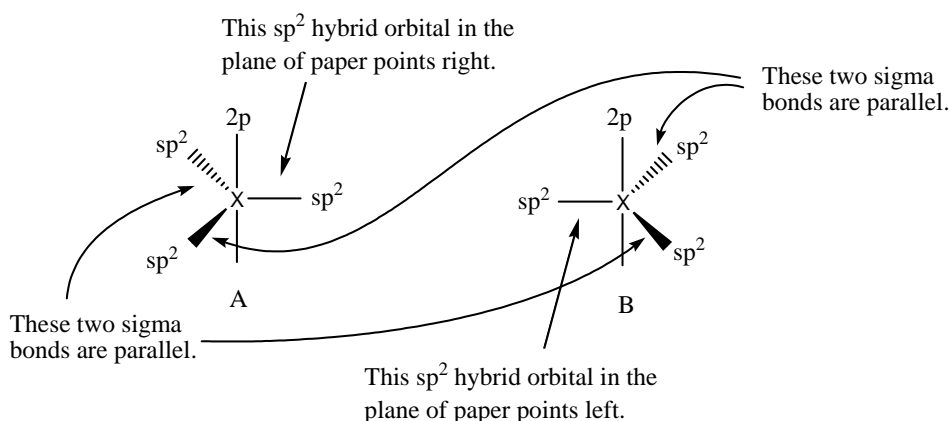
1. If a triple bond or an aromatic ring is present in your 2D Lewis structure, it is often easier to begin first with one of these, or both if you can do it. If you draw an aromatic ring, draw it big so the lower lobes of the p orbitals in the back do not overlap the top lobes of the p orbitals in the front.



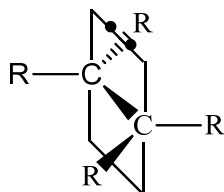
2. There are many types of double bonds possible. These pi bonds are drawn in the plane of the page, but they can be drawn in and out of the page too. Some pi bond possibilities include: $C=C$, $C=N$, $C=O$, $C=F^+$, $-N=O$, $-N=N-$ and $O=O$.

There are only two possible shapes for an sp^2 hybridized atom, if the pi bond is drawn in the plane of the paper. Look for the parallel bond relationships in any attached sp^2 or sp hybridized atoms to decide if lines are dashes, wedges or simple and which way they point. Pi bonds can be drawn in the plane, coming out of the plane or projecting behind the plane of view. Every sp^2 atom has three side orbitals (the hybrid orbitals) and a perpendicular p orbital to that plane. Those three side sp^2

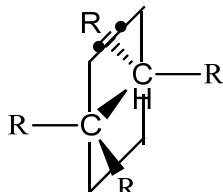
orbitals will each have a parallel sp^2 orbital in other trigonal planar atoms. Use these as your guide when continuing a sequence of attached atoms.



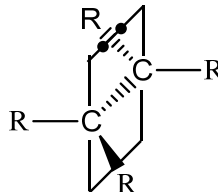
pi bond drawn sideways, parallel to the plane of the paper



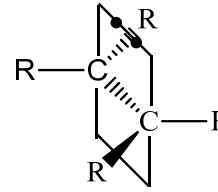
pi bond drawn projecting out of the plane of the paper, left carbon drawn first



pi bond drawn projecting out of the plane of the paper, right carbon drawn first



pi bond drawn projecting behind the plane of the paper, left carbon drawn first

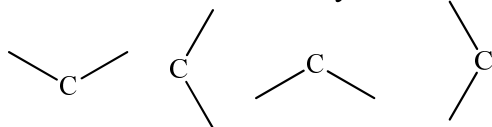


pi bond drawn projecting behind the plane of the paper, right carbon drawn first

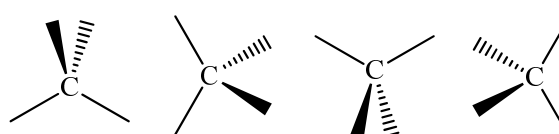
3. Pi bonds can be joined together in an almost endless number of possible ways. (two triples, triple plus a double, two doubles, cumulated, aromatic...etc.). Examples are in the topic notes.

4. Sp^3 hybridization may be the most difficult to represent in three dimensions. Simple single bonds allow unlimited rotations. To make your drawing easier assume that tetrahedral atoms are in a zig-zag conformation (shape) in the plane of the paper. Extending a chain horizontally across a page is usually easiest. We will typically try to draw two simple lines, in the plane of the paper and one wedged line (in front) and one dashed line (behind). The two simple lines will have to be drawn close to one another, as will the dashed and wedged lines. These can be difficult to draw accurately and we will allow shapes to be drawn that are "pretty close". Once you draw a wedge and a dash you establish a viewing perspective, either from the left or from the right. You should try to keep that perspective as you draw your other atoms.

These lines are drawn correctly.

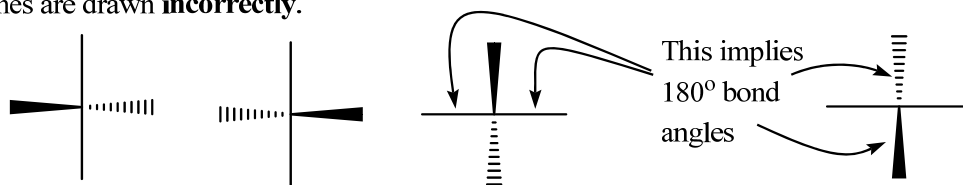


Simple lines can be drawn close together four different ways, pointing up, pointing right, pointing down and pointing left.

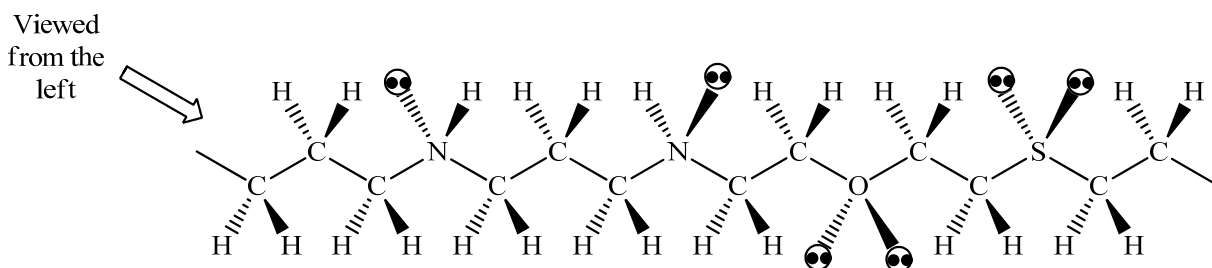
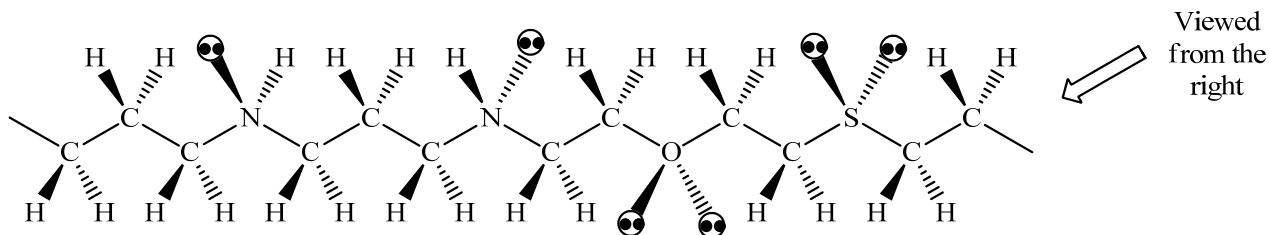


Wedged and dashed lines can be drawn close together four different ways, pointing up, pointing right, pointing down and pointing left.

These lines are drawn **incorrectly**.



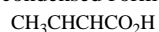
Drawing the simple lines or the wedged and dashed lines opposite one another implies that there are 180° bond angles...but we know that sp^3 atoms have approximately 109° bond angles.



Simple functional group examples that you are responsible for.

1. Carboxylic acids

condensed formula



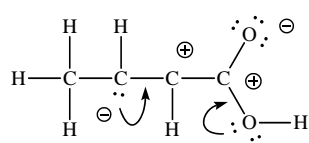
$$4 \times \text{C} = 16 \text{ e}^-$$

$$6 \times \text{H} = 6 \text{ e}^-$$

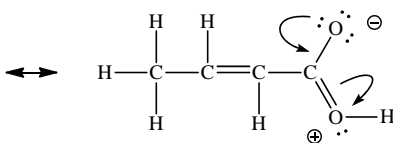
$$2 \times \text{O} = 12 \text{ e}^-$$

$$\text{total} = 34 \text{ e}^-$$

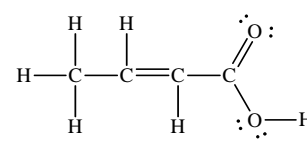
2D formula



starting structure = poor

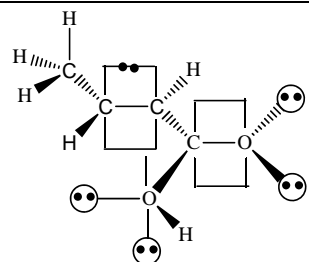


= 2



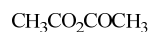
best = 1

3D formula
of best

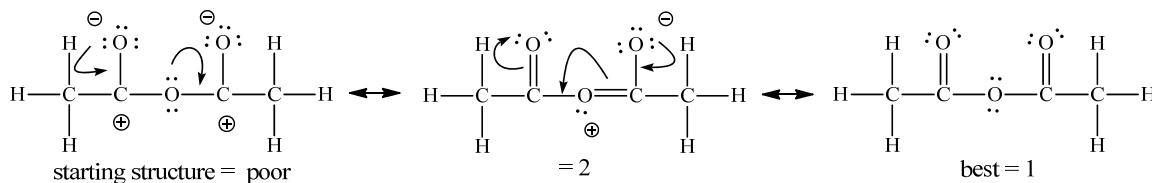
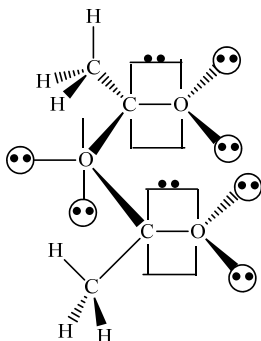


2. Anhydride

condensed formula

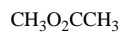


$$\begin{aligned} 4 \times \text{C} &= 16 \text{ e}^- \\ 6 \times \text{H} &= 6 \text{ e}^- \\ 3 \times \text{O} &= 18 \text{ e}^- \\ \text{total} &= 40 \text{ e}^- \end{aligned}$$

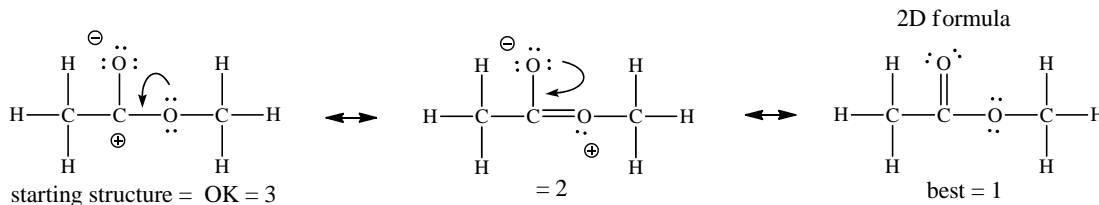
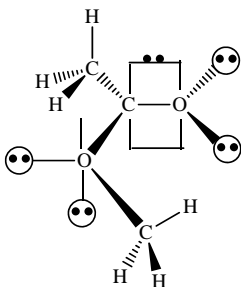
3D formula
of best

3. Ester

condensed formula



$$\begin{aligned} 5 \times \text{C} &= 20 \text{ e}^- \\ 6 \times \text{H} &= 6 \text{ e}^- \\ 2 \times \text{O} &= 12 \text{ e}^- \\ \text{total} &= 38 \text{ e}^- \end{aligned}$$

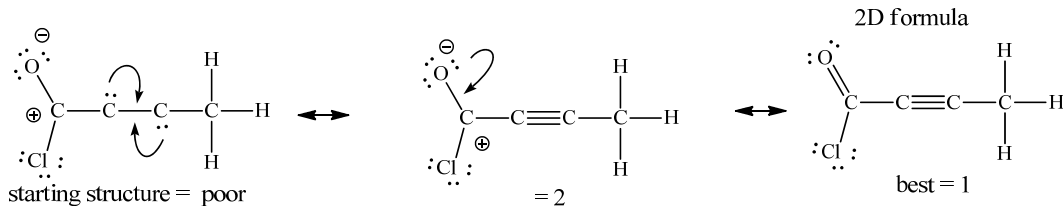
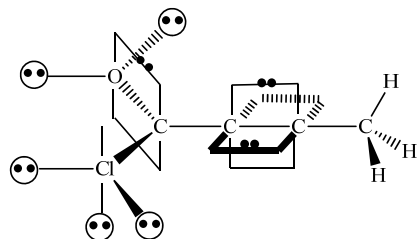
3D formula
of best

4. Acid chloride

condensed formula



$$\begin{aligned} 4 \times \text{C} &= 16 \text{ e}^- \\ 3 \times \text{H} &= 3 \text{ e}^- \\ 1 \times \text{O} &= 6 \text{ e}^- \\ 1 \times \text{Cl} &= 7 \text{ e}^- \\ \text{total} &= 32 \text{ e}^- \end{aligned}$$

3D formula
of best

5. Amides

condensed formula



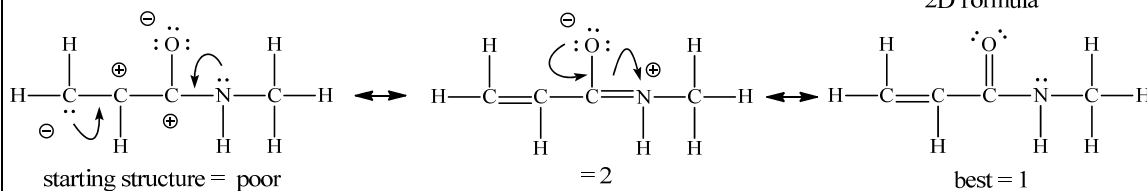
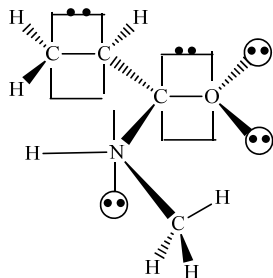
$4 \times \text{C} = 16 \text{ e}^-$

$7 \times \text{H} = 7 \text{ e}^-$

$1 \times \text{O} = 6 \text{ e}^-$

$1 \times \text{N} = 5 \text{ e}^-$

total = 34 e⁻

3D formula
of best

6. Nitriles

condensed formula

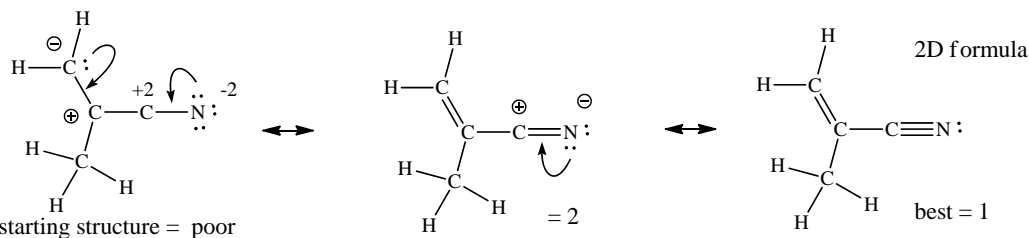


$4 \times \text{C} = 16 \text{ e}^-$

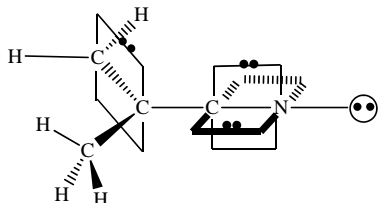
$5 \times \text{H} = 5 \text{ e}^-$

$1 \times \text{N} = 5 \text{ e}^-$

total = 26 e⁻

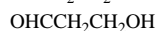


3D formula



7. Aldehydes (and an alcohol)

condensed formula

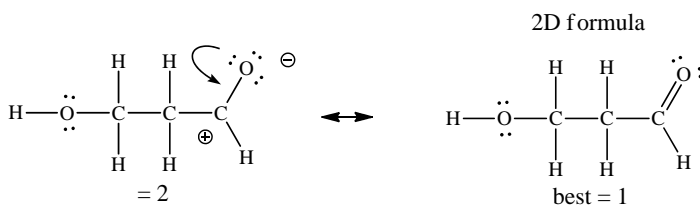


$4 \times \text{C} = 16 \text{ e}^-$

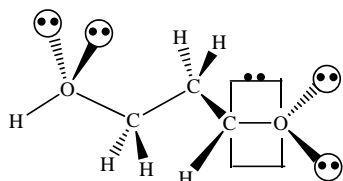
$6 \times \text{H} = 6 \text{ e}^-$

$2 \times \text{O} = 10 \text{ e}^-$

total = 32 e⁻



3D formula



8. Ketones

condensed formula

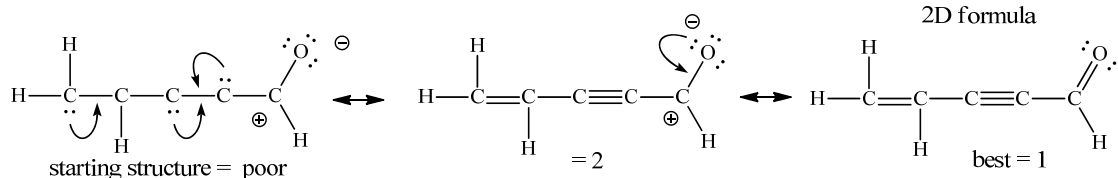
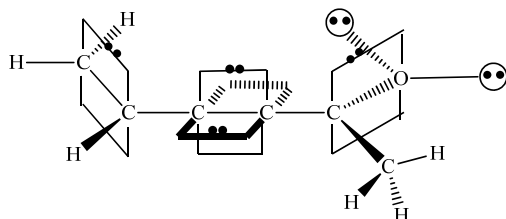


$6 \times \text{C} = 24 \text{ e}^-$

$6 \times \text{H} = 6 \text{ e}^-$

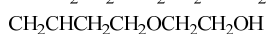
$1 \times \text{O} = 6 \text{ e}^-$

total = 32 e⁻

3D formula
of best

9. Alcohols

condensed formula

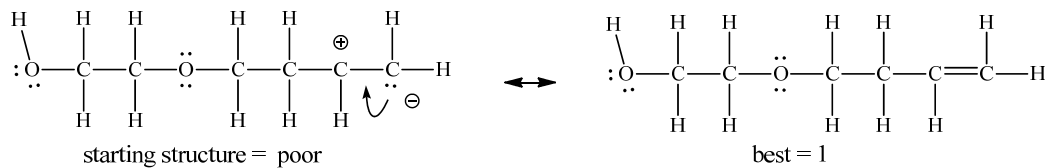
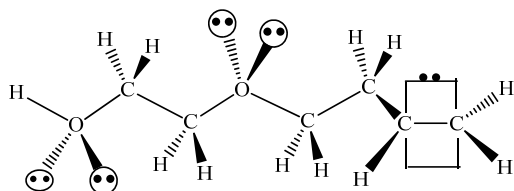


$6 \times \text{C} = 24 \text{ e}^-$

$12 \times \text{H} = 12 \text{ e}^-$

$2 \times \text{O} = 12 \text{ e}^-$

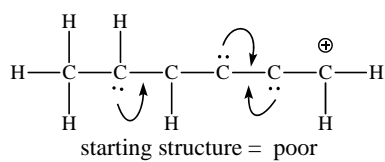
total = 48 e⁻

3D formula
of best

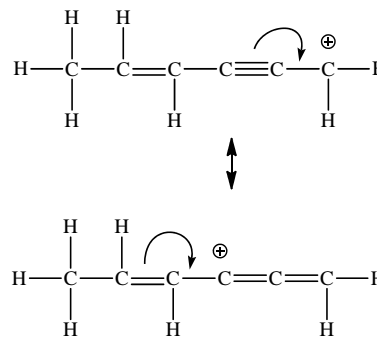
condensed formula



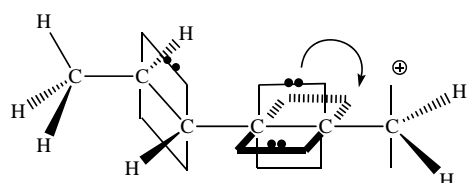
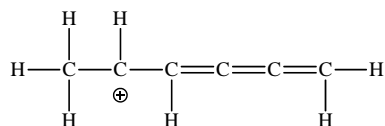
$$\begin{aligned} 6 \times \text{C} &= 24e^- \\ 7 \times \text{H} &= 7e^- \\ \oplus &= -1e^- \\ \text{total} &= 30e^- \end{aligned}$$



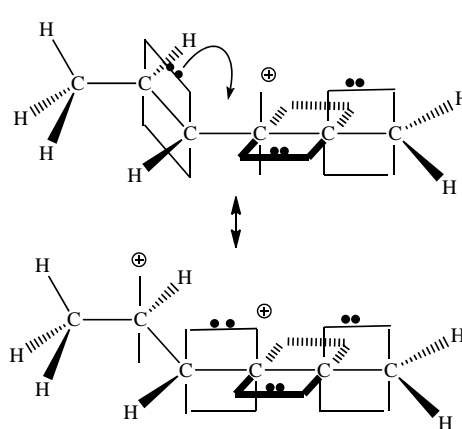
2D formula



cation



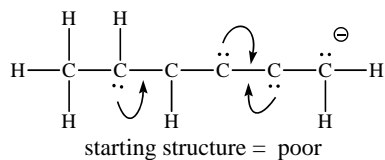
3D formula



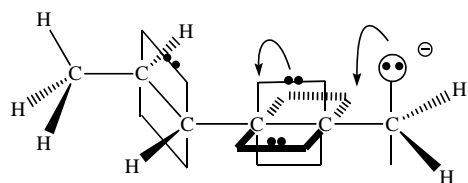
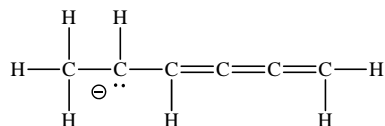
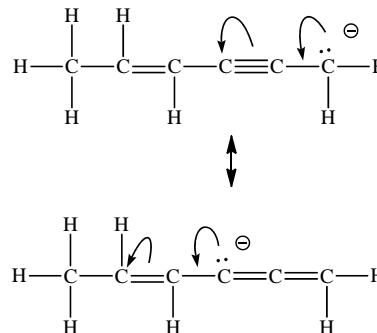
condensed formula



$$\begin{aligned} 6 \times \text{C} &= 24e^- \\ 7 \times \text{H} &= 7e^- \\ \ominus &= +1e^- \\ \text{total} &= 32e^- \end{aligned}$$



2D formula



3D formula

