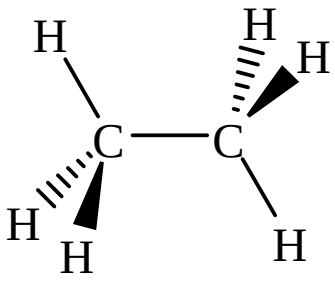
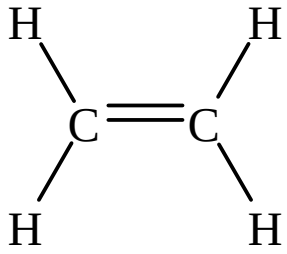
Structure and Nomenclature

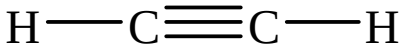
Stable carbon-containing compounds have four bonds to carbon.



ethane

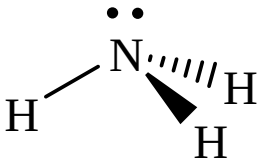


ethene
(ethylene)

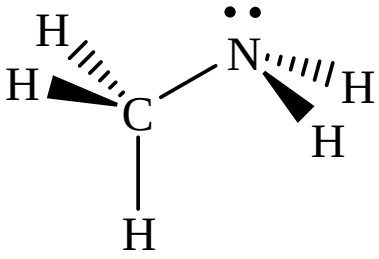


ethyne
(acetylene)

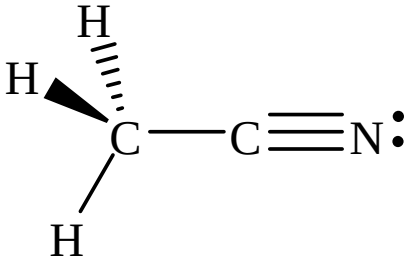
Three bonds to nitrogen...



ammonia

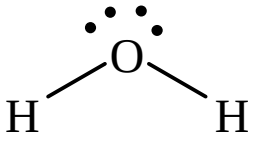


aminomethane
(methylamine)

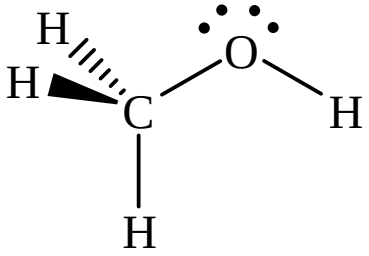


acetonitrile

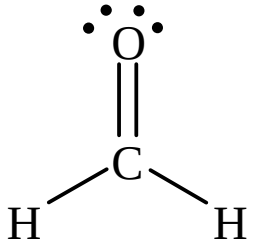
Two bonds to oxygen...



water

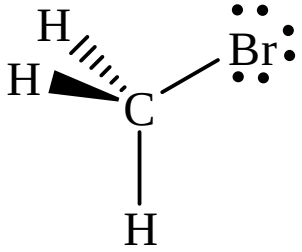


methanol

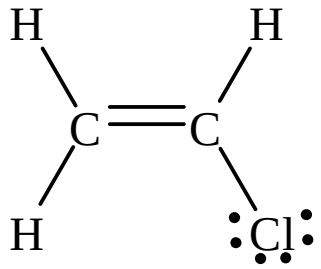


formaldehyde

One bond to H, F, Cl, Br, I...



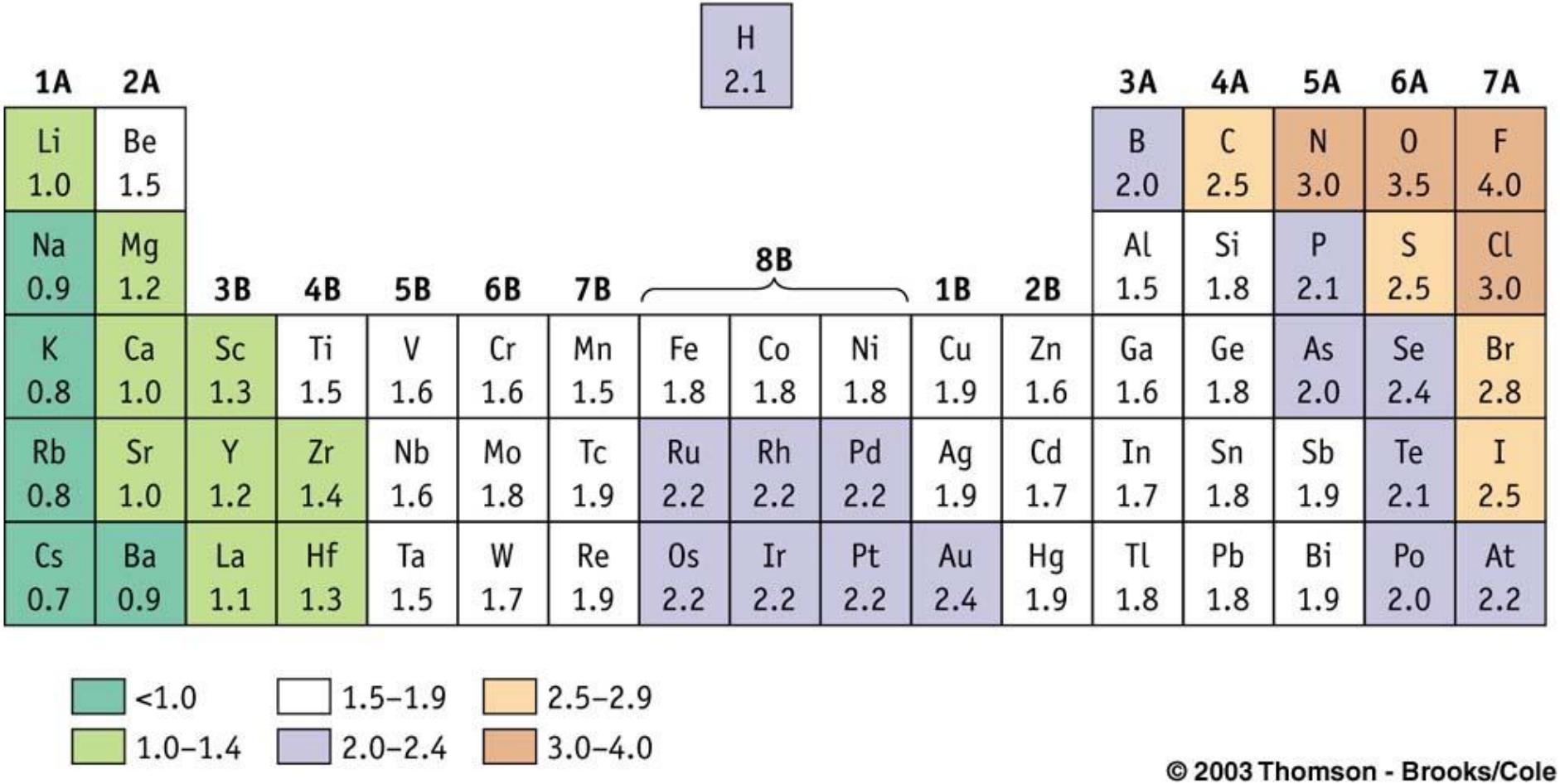
bromomethane



chloroethene
(vinyl chloride)

Developing Reasonable Lewis Structures for Organic Molecules

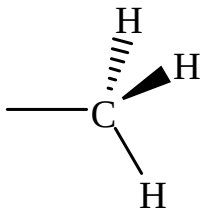
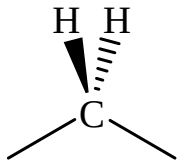
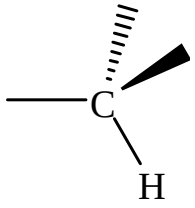
1) Draw the full structure of the molecules with the connectivity suggested by the formula such that all valences are met (octets for C, N, O, F, Cl, Br, I).
2) Always show all valence shell electrons (including lone pairs)
   a) Count the number of valence electrons in the entire molecule (each atom has the same number of valence electrons as its group number in the periodic table).
   b) From the number in a, subtract the number of bonding electrons (2 times the # of lines in your structure). Any electrons that are unplaced are added to atoms that lack a full octet (usually heteroatoms) as lone pairs.
   c) Atoms still lacking octets are completed using lone pairs from adjacent atoms to form multiple bonds.
3) Always show formal charges according to the following formula:
   FC = # of valence electrons – (# of bonds to that atom) – (# of lone pair electrons)
4) Never draw structures with adjacent like charges.
5) Formal charges of 0 is always better than charge separation.
6) Do not place multiple charges on 1^{st} or 2^{nd} row atoms (+1 or -1 only), and try to avoid charges altogether (a neutral structure is always best).
7) Always place – charges on the more electronegative atom and + charges on the less electronegative atom.
8) Do not place charges on carbon if the overall molecule is neutral.
9) In general, H only needs 2 electrons, B and Al need only 6 electrons, and atoms below the second row may have more than 8 electrons.
10) Try to avoid O-O bonds.



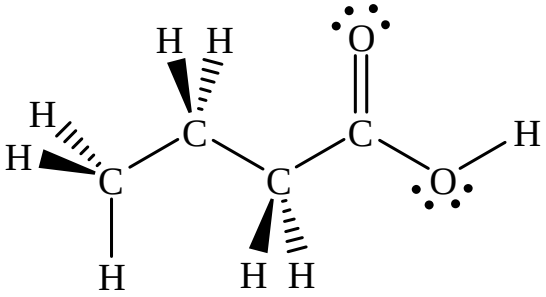
The periodic trend in Pauling's electronegativity...

Drawing Organic molecules - Condensed and Line Structures.

Hydrocarbon fragments:

Name	Expanded form	Condensed form
methyl		—CH_3
methylene		—CH_2—
methine		—CH

Writing condensed structures…

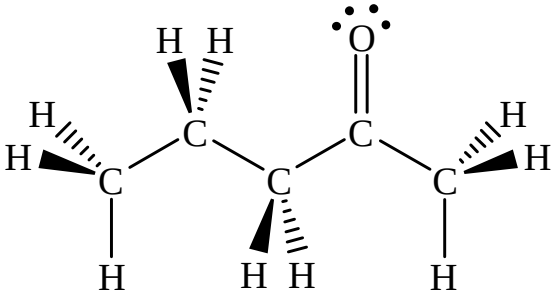


Full Structure (expanded form)

The condensed form of most functional groups is written backwards if the group is found on the left hand side of the structure...

$H—O—CH_2—CH_3$ → $HOCH_2CH_3$ not $OHCH_2CH_3$

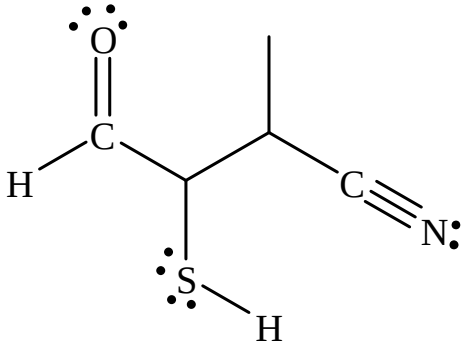
Writing line structures…

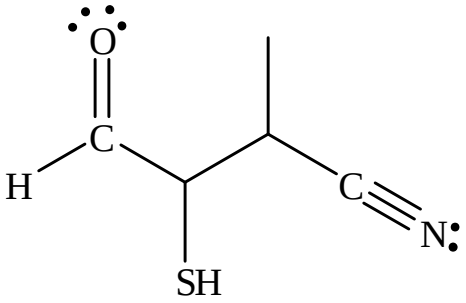


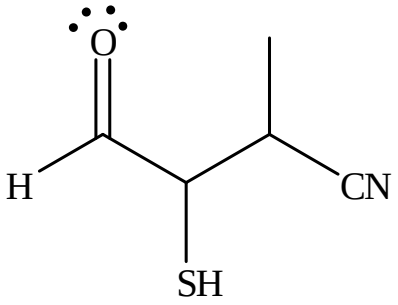
Expanded Structure

When drawing line structures:

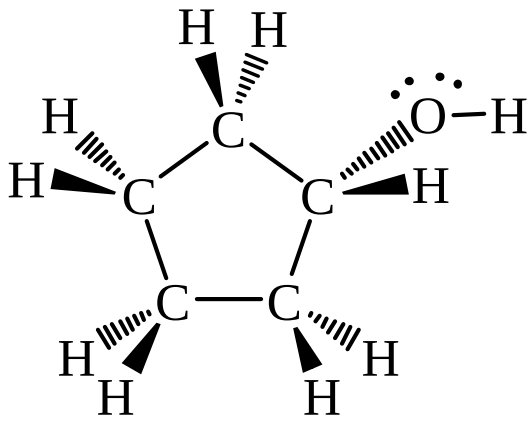
- use lines to represent carbon-carbon bonds.
- ignore carbon-hydrogen bonds in *hydrocarbon units*.
- *always* draw heteroatoms and hydrogen atoms attached to heteroatoms.
- draw all the atoms for functional groups (for the most part).

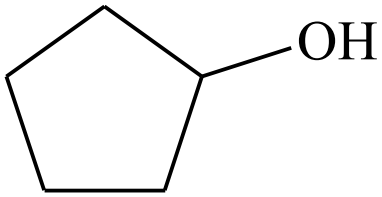


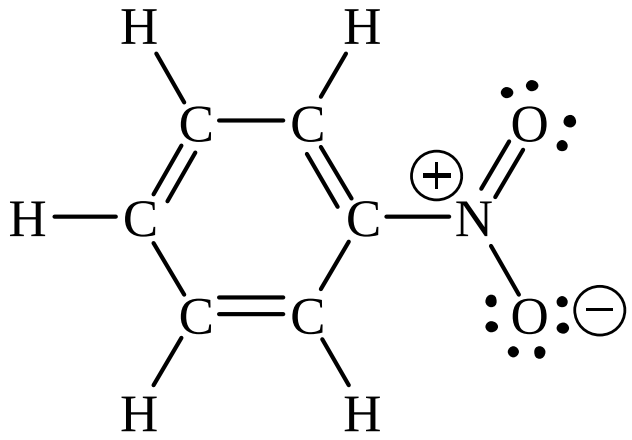


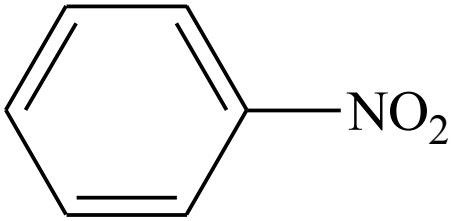


Line structures are very useful for cyclic molecules



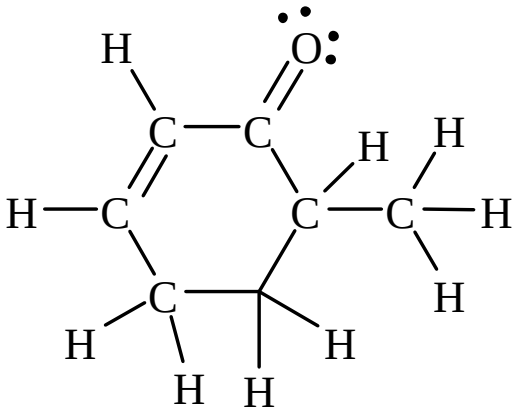


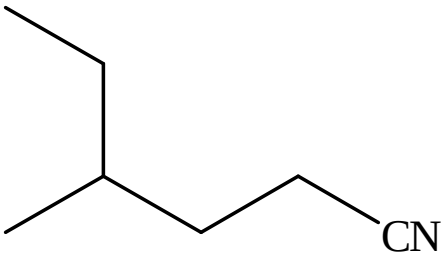




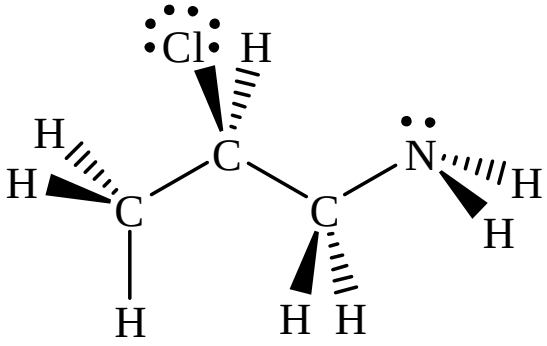
These examples demonstrate how ‘clean’ line structures look compared to expanded or even condensed structures.

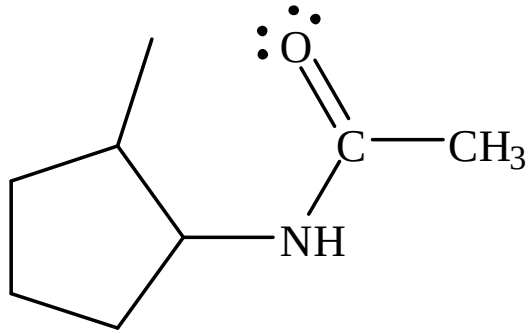
Practice!



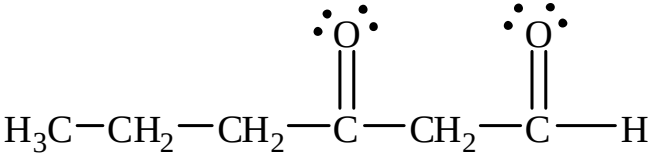


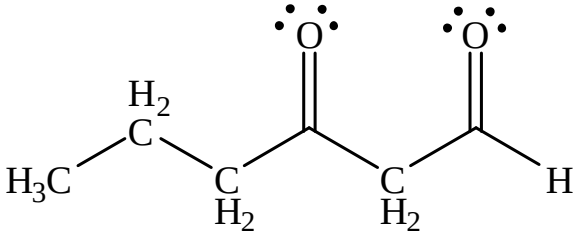
Practice!



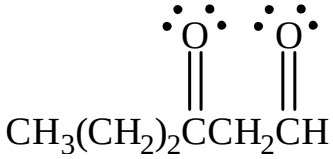


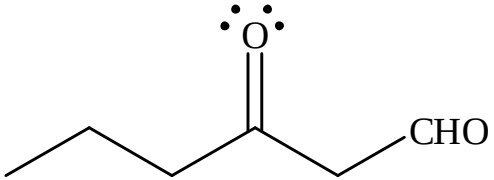
Ultimately, organic molecules are usually drawn as a mixture of expanded, condensed, and line structures. Be careful however, molecules can be drawn many different ways and look completely different...

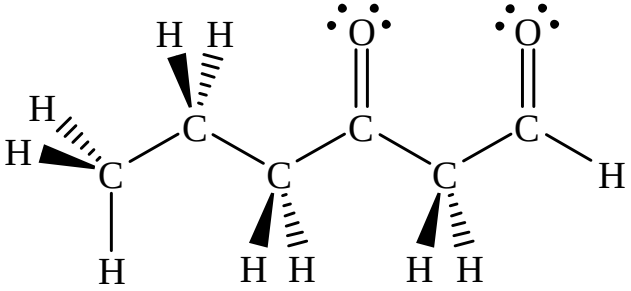


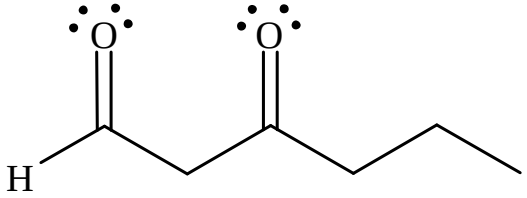


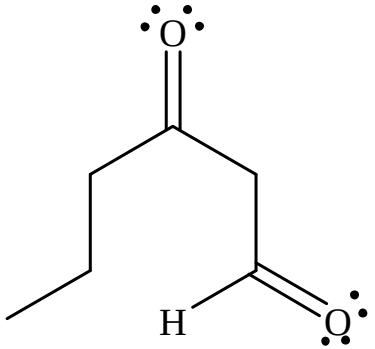
$CH_3CH_2CH_2COCH_2CHO$











Warnings:

- The end of a line represents a methyl group *not* a hydrogen atom.
- If you draw 'C', you *must* draw all atoms attached to it.

For most (neutral) organic compounds, Lewis structures can be determined simply by taking the connectivity implied (remember that there are 4 bonds to carbon, 3 to nitrogen, 2 to oxygen and 1 to hydrogen) and filling the octets.

$HCONH_2$

H_2NCONH_2

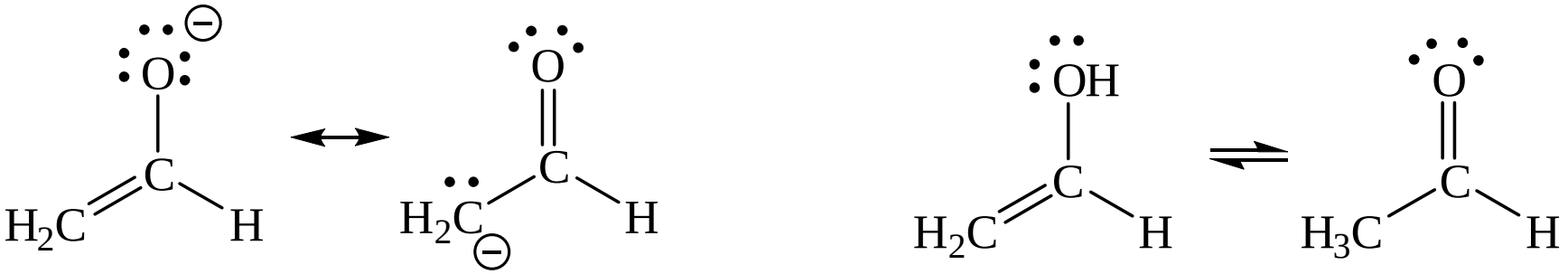
$(CH_3O)_2CH^+$

$[CH_2CHCH_2]^+$

Rules for Drawing and Interpreting Resonance Structures

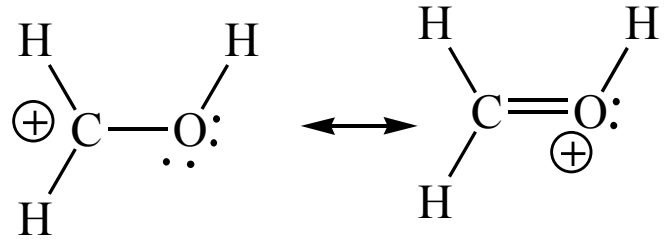
Resonance structures show how electrons are delocalized within a species. When drawing and evaluating resonance structures, it is important to keep track of any and all lone pairs (unshared electron pairs).

1. Only lone pair electrons and multiple-bond electrons (pi-electrons) move from one resonance structure to another. Atoms never move.

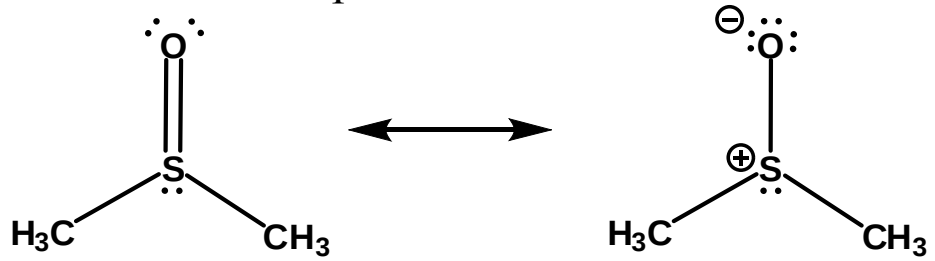


2) From structure to structure, electron pairs move in the following ways:

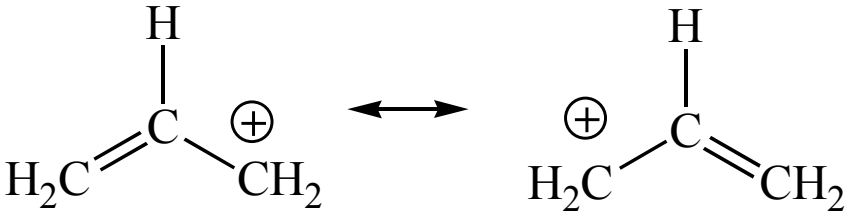
lone pair to form an adjacent bond:



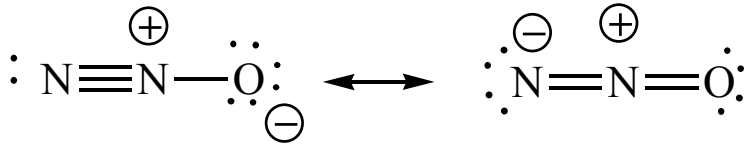
bond to form a lone pair:



bond to form a new bond:

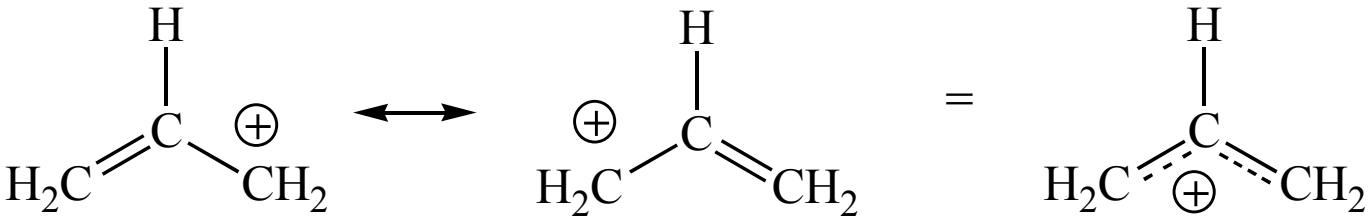


3) Electrons move only to adjacent positions, but more than one pair of electrons can move from one structure to another.



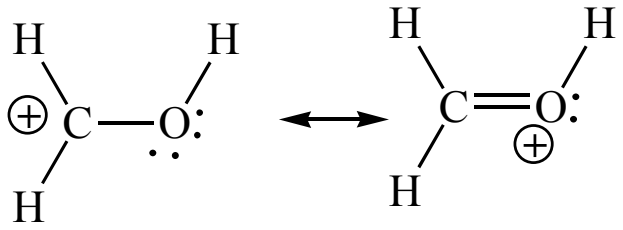
4) Always check to see what happens to the formal charges on specific atoms. The net charge on each structure must be the same.

5) Structures that are identical in form are said to be degenerate. Such structures contribute the same to the overall structure. Resonce "hybrids" are often drawn of such structures.

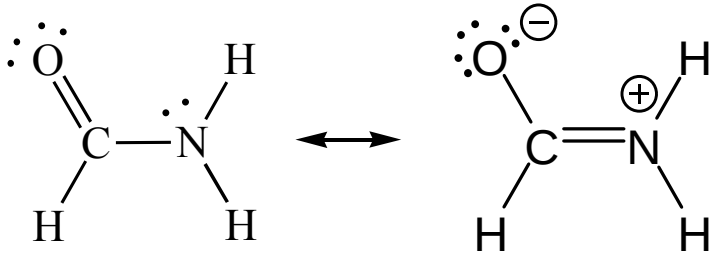


6) When resonance structures are not degenerate, use the following rules to judge which structures contribute more to the character of the species:

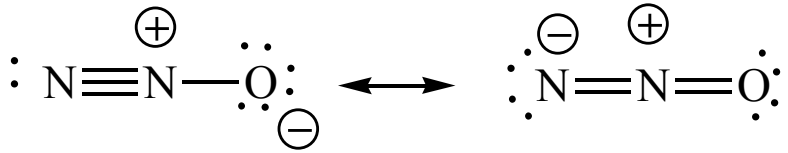
i) Resonance structures in which second period atoms (C-F) all have octets are favoured over those with electon deficient atoms--resonance structures that have more than 8 electrons on such atoms are not valid.



ii) When comparing resonance structures with the same number of bonds, structures with fewer formal charges contribute more to the character of a species

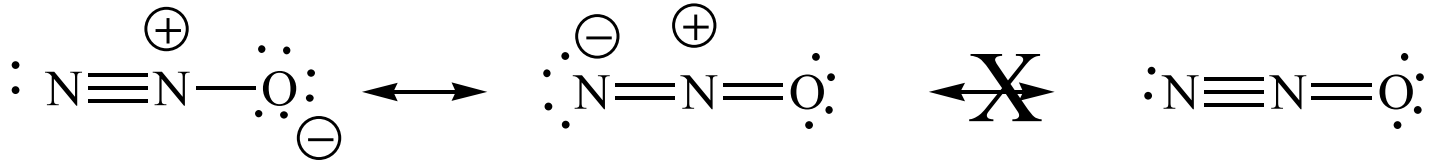


iii) In cases where there are resonance structures with the same number of formal charges, the favoured structure will be that in which the negative charge is on the more electronegative atom or positive charge is on the more electropositive element.

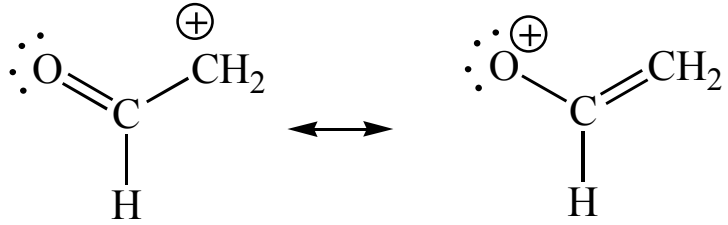


Invalid Resonance Structures (Fatal Flaws which result in a 0!)

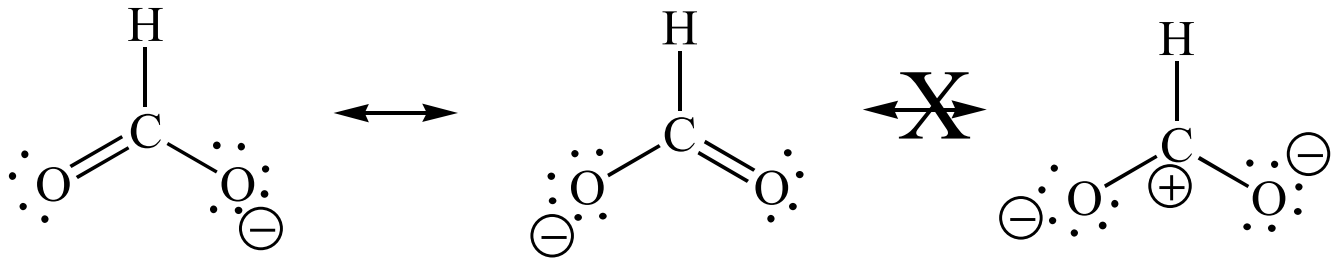
i) have more than eight electrons on a second row element



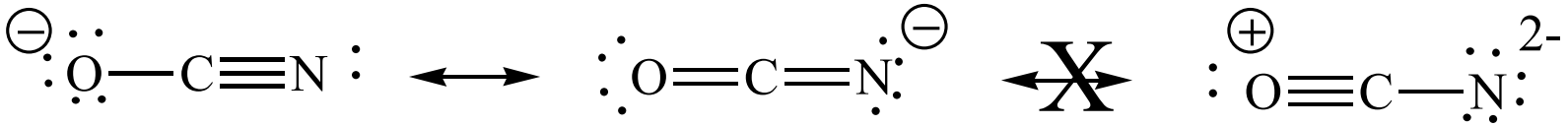
ii) have less than eight electrons on O or N (or similarly electronegative element)



iii) have more than two atoms bearing formal charges (except polynitros and a few others)



iv) have any 2nd row atom with a formal charge greater than +/-1 (except S).



$HCO_2^{\ominus}$ CH_3NO_2 H_2CN_2 $HCONH_2$

benzene