General Rules for Constructing Dot Structures

1. Determine the number of valence electrons.

2. Connect atoms using single bonds.

3. Add remaining electrons up to an octet (except hydrogen), starting with the terminal atoms.

4a. For atoms that do not have a full octet, move lone pairs to form multiple bonds such that the octet rule is satisfied for all atoms (if possible).*

4b. You may exceed the octet rule for central atoms that have low-lying empty d orbitals (Si, P, S, Cl, Ge, As, Se, Br, Sb, Te, I).

4c. In general the best dot structure will be the one that:

1st, minimizes formal charge;

2nd, places negative formal charges on the most electronegative atoms, and positive formal charge on the least electronegative atoms; and

3rd, places opposite formal charges as close together as possible, and separates like formal charges as much as possible

*Note: there are rare exceptions to rule 4a. The classic example is BF_3, where making a double bond between boron and fluorine would place a positive formal charge on fluorine and a negative formal charge on boron which would be expected to be much disfavored based on electronegativity

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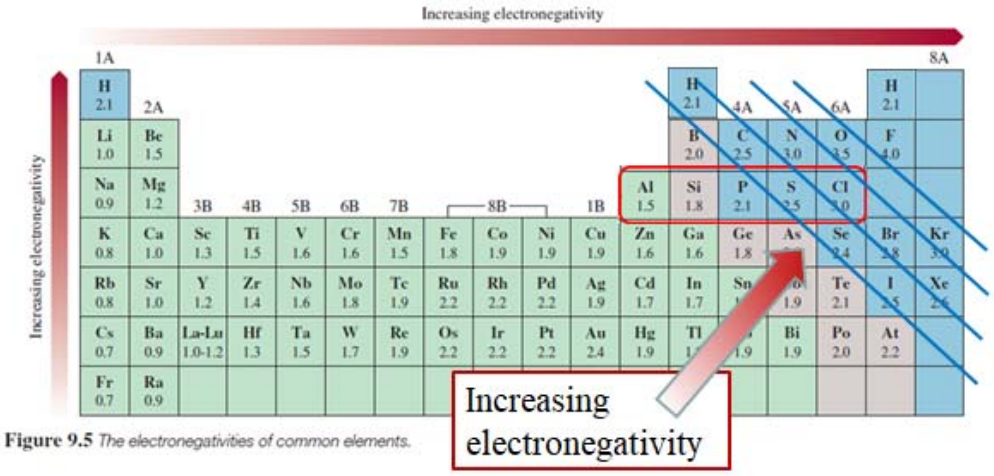

Figure 9.5 *The electronegativities of common elements.*

Special cases: (1) EN(O) > EN(Cl)
(2) EN(H) ≈ EN(C)

Electron Accounting Systems

# e^- atom has	=	# e^- atom should have	–	# e^- atom actually has
	=	# valence e^-	–	{# lone pair e^- + # bonding e^- that "belong" to the atom}
oxidation number, ON (assumes 100% ionic)	=	# valence e^-	–	{# lone pair e^- + # bonding e^-} giving all to the most EN atom
formal charge, FC (assumes 100% covalent)	=	# valence e^-	–	{# lone pair e^- + # bonding e^-} split evenly between the atoms

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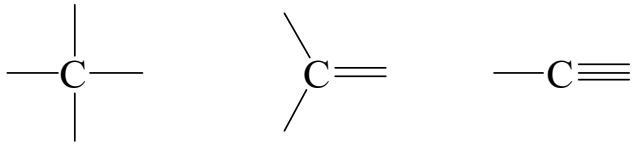
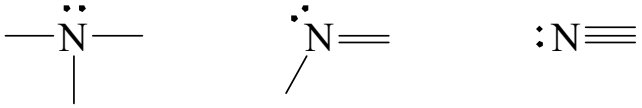
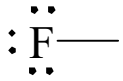
To have zero formal charge (FC) on an atom:

atom	# bonds	# lone pairs	examples
C	4	0	
N	3	1	
O	2	2	
F	1	3	

Increasing # bonds and decreasing # lone pairs by one ⇒ increase FC by one.

Decreasing # bonds and increasing # lone pairs by one ⇒ decrease FC by one.

Important and common examples:

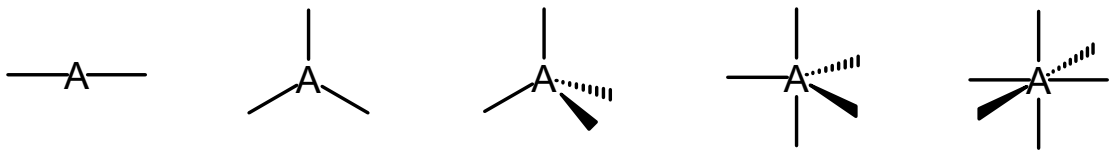
Dot Structure and Molecular Geometry (VSEPR) Practice Set

For each of the following molecules/ions, draw the best dot structure for each species in the boxes provided below, and show all nonzero formal charges.

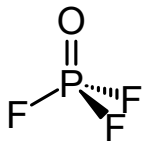
AsH_3	SF_6	BrF_5	$AlCl_4^-$
SF_3^-	SCl_2	ClO_3^-	HCN
I_3^-	SOO	IF_4^+	XeF_4

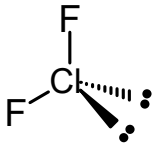
Now determine the molecular shape of each species (the shape formed by the atoms, as if the lone pairs were "invisible"). Do not just give the name of the molecular shape (e.g. linear, bent, T-shaped, trigonal planar, trigonal pyramidal, tetrahedral, trigonal bipyramidal, distorted tetrahedron/"seesaw", square planar, square pyramidal, or octahedral), but also sketch the shape. As we discussed in class, use wedges to show bonds coming out of the plane of paper (towards you) and dashed lines for bonds going into the plane of the paper (away from you).

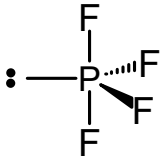
It takes some practice to get the hang of this, and it helps if you use the same basic templates each time, such as shown below.



For example, using these templates, the VSEPR sketches for $O\underline{P}F_3$, ClF_2^+, and PF_4^- (ignoring distortions from ideal) would be







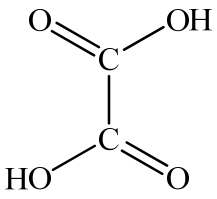
Sketch the molecules and ions on from the previous page using wedges and dashed lines to show the molecular geometry, and write the name for that geometry.

name: _____	name: _____	name: _____	name: _____
name: _____	name: _____	name: _____	name: _____
name: _____	name: _____	name: _____	name: _____

Which of the above neutral molecules would be polar?

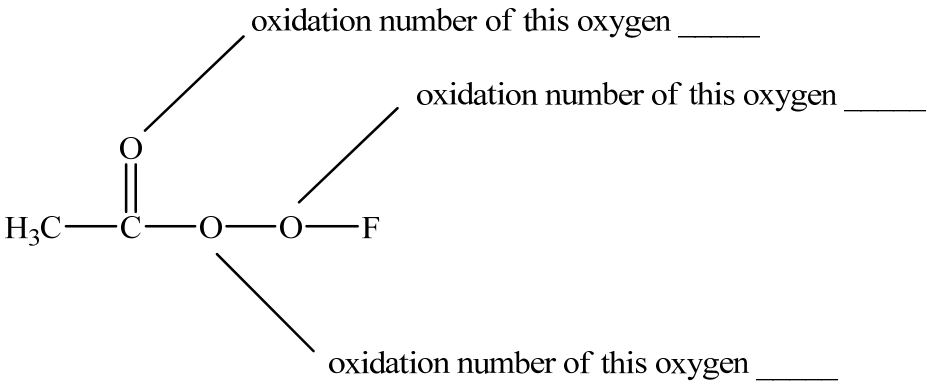
Practice Exercise: Oxidation Numbers

Assign oxidation numbers for the atoms identified below:

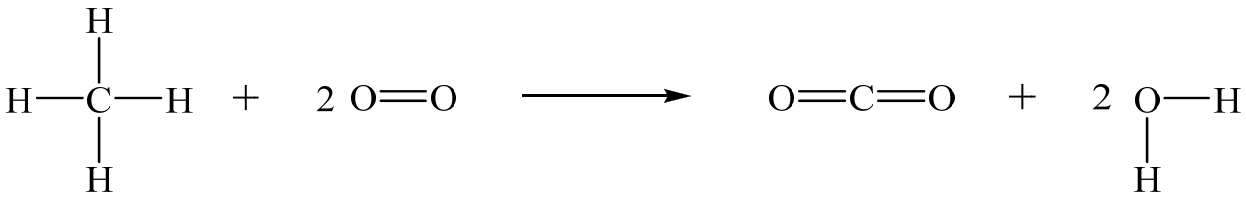


oxidation number of carbon _____

H_3CNC oxidation number of the carbon on the right _____



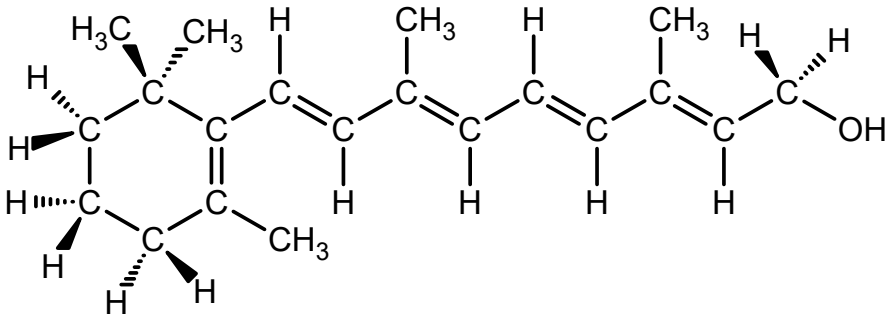
Assign the oxidation numbers for all of the atoms in each of the species in the following chemical equation. (Lone pairs are not shown, but do not forget to consider them when you assign the oxidation numbers.)



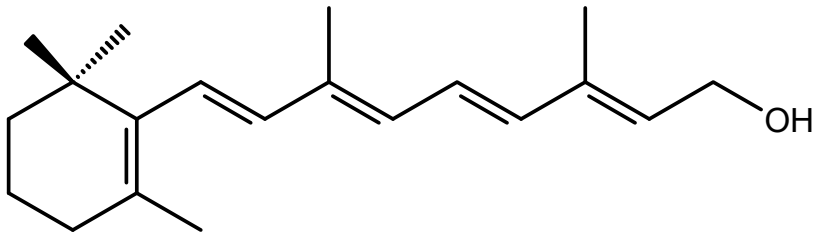
Line Drawing for Representing Hydrocarbon Structures

One of the important properties of carbon is its ability to form large molecules based on extended carbon-carbon bonds. Such molecules are very important in biology and industry, and we need an efficient and generally recognized way to represent them. The convention is to draw large hydrocarbons such that each vertex and terminus represents a carbon atom. Since carbon usually has four bonds, four minus the number of bonds to a given carbon gives the number of hydrogen atoms bonded to that carbon. Organic chemists call these representations "line drawings."

For example, vitamin A

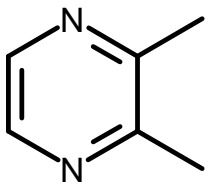


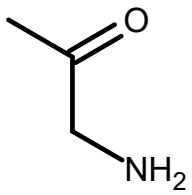
can be equivalently represented as

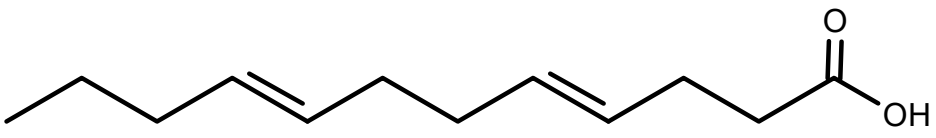


and either structure gives the formula $C_{20}H_{30}O$. (The formulas of organic compounds are generally written as C_xH_y followed by the remaining elements in alphabetical order.)

Give the formula for each of the following structures.







More line drawing practice...

Compounds known to contribute to the sensory perception of wine flavor. Note how the senses of smell and taste are combined in describing the role of these compounds.

http://pubs.rsc.org/en/content/articlehtml/2008/cs/b714455p