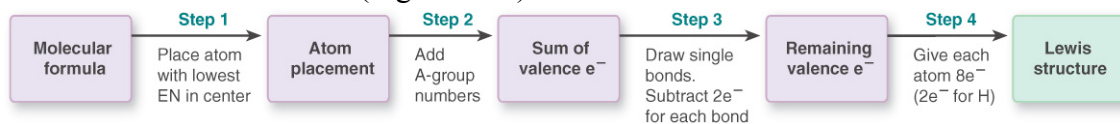


Overview of Chapters 10 & 11

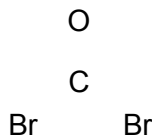
Theory of Covalent Bonding

Starting with the molecular formula for a covalently bonded molecule or polyatomic ion it is possible to predict a wide range of molecular properties by applying a few simple procedures. These include drawing the Lewis structure to determine the distribution of electrons about the central atom, applying the VSEPR theory to predict the electron geometry and molecular shape of the molecule, using formal charges to predict the most probable resonance structure for a molecule if there are multiple ones to choose from, and using electronegativity values to predict molecular polarity. The electron geometry can also be used to predict the hybridization of the atomic orbitals and the types of covalent bonds (σ and π) that are used to bond the atoms together. Below is an example of apply these procedures to a molecule of COBr_2

A. Draw the Lewis structure (Figure 10.1)



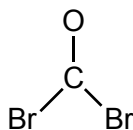
- Step 1:* The carbon has the lowest electronegativity, so it will be placed in the center:



- Step 2:* Count up the valence shell electrons using the A-group numbers fore each atom:

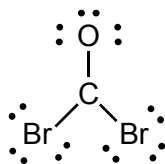
Atom	Group	Valence electrons
C	4A	+4 e's
O	6A	+6 e's
Br	7A	+7 e's
Br	7A	+7 e's
Net Charge	0	+0 e's
Total Valence e's		+24 e's

3. *Step 3:* Connect the atoms with single bonds, and subtract a pair of valence electrons from the total for each bond:

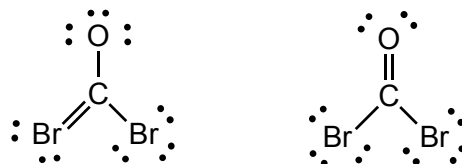


- a. $24 \text{ e}'\text{s} - 3(2 \text{ e}'\text{s}) = 18 \text{ e}'\text{s}$ remaining.

4. *Step 4:* Distribute the remaining valence electrons in pairs, starting with the surrounding atoms, giving each 8 e's, until all of the valence electrons are used up:

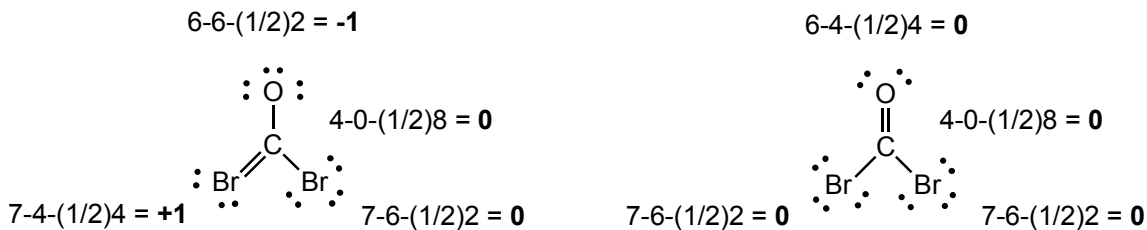


- a. At this point, each of the surrounding atoms has 8 valence electrons, however, the central carbon atoms only has 6. This situation is remedied by making a multiple bond.
5. *Step 5:* If after distributing the remaining valence electrons, the central atom has fewer than 8 valence electrons, bring in a pair of lone pair electrons from one of the surrounding atoms and form a multiple bond.
- a. For this molecule, there are two possible structures:



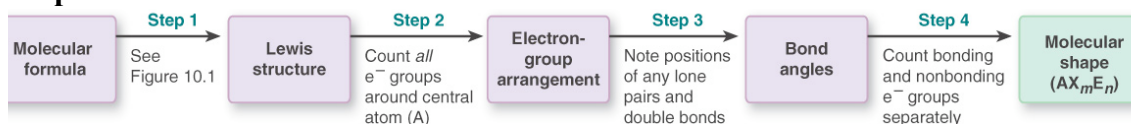
B. Determine the more probable resonance

1. The more probable resonance structure can be predicted by the determining the formal charges for each of the atoms in each structure.
- a. Formal charges are determined by subtracting from the group number for each atom, the number of lone pair electrons and the 1/2 the number of bonding electrons.

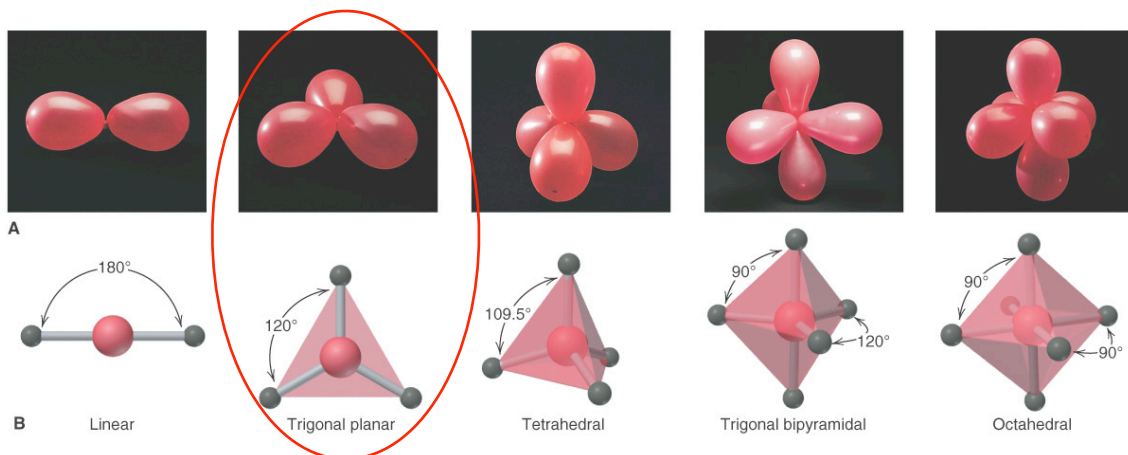


2. The structure on the right has the smallest set of formal charges, making it the more probable structure.

C. Applying the VSEPR theory to determine the electron geometry and the molecular shape.

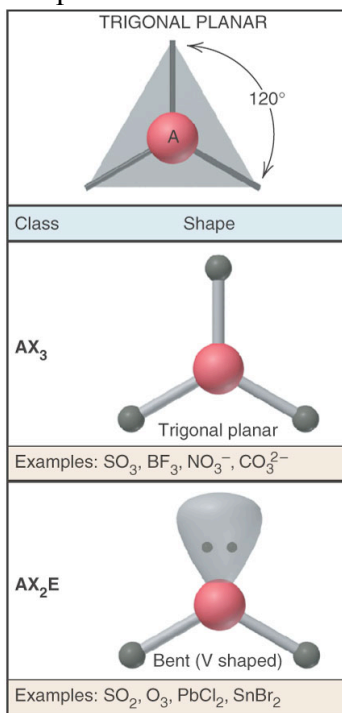


1. *Step 1:* Draw Lewis structure, done.
2. *Step 2:* Count the e^- groups
 - a. 2 single bonds, 1 double bond, and no lone pairs = 3 e^- groups.
 - b. 3 groups of electrons gives a trigonal planar electron geometry:



3. *Step 3:* Determine the bond angles:
 - a. For trigonal planar geometry, the ideal VSEPR bond angle is 120° . Lone pairs and double bonds, which require more space, will distort the bond angles from the ideal angle. Since COBr_2 has a double bond, we expect the $\text{Br}-\text{C}-\text{Br}$ angle to be slightly less than 120° and the $\text{Br}-\text{C}-\text{O}$ angles to be slightly greater than 120° .

4. *Step 4: Determine the molecular shape.*
- a. This is done ignoring the lone pairs of electrons and observing the resulting shape. For trigonal planar electron-group geometry there are two possibilities:
- Trigonal planar if there are no lone pairs of electrons.
 - Bent, if there is one pair of lone electrons.



- b. Since $COBr_2$ has no lone pairs of electrons, it has a trigonal planar molecular geometry.

D. Determine molecular polarity

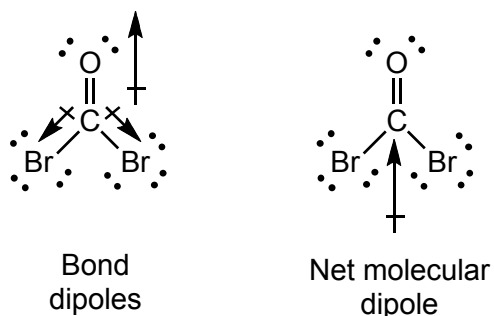
1. First determine if there are any polar covalent bonds by comparing electronegativities:

Atom	EN
C	2.5
O	3.5
Br	2.8

2. The bond polarities are determined by look at the differences in electronegativity for each bond, ΔEN .

Bond	ΔEN
C=O	1
C-Br	0.3

- a. The C=O bond is polar, whereas the C-Br bonds are only slightly polar. Eventhough the C-Br bonds are in arrangement that allows them the partilly reduce the polarity of the C=O bond, the molecule will have a net dipole:



E. Determine the atomic orbital hybridization for the central atom.

1. The number of atomic orbitals that must hybridized for a given electron-group geometry is equal to the number of electron-groups in a given geometry

e-group geometry	No. of e-group	<i>s</i>	<i>p</i>	<i>d</i>	Hybrid Orbitals
Linear	2	1	1		2 <i>sp</i> Orbitals
Trigonal Planar	3	1	2		3 <i>sp</i> ² Orbitals
Tetrahedral	4	1	3		4 <i>sp</i> ³ Orbitals
Trigonal Bipyramidal	5	1	3	1	5 <i>sp</i> ³ <i>d</i> Orbitals
Octahedral	6	1	3	2	6 <i>sp</i> ³ <i>d</i> ² Orbitals

2. Given that the electron-group geometry of COBr₂ is trigonal planar, the hybridization of the central carbon is *sp*².

F. **Determine the bonding types**

1. The COBr_2 has three bonds, 2 single bonds between the central carbon atom and the two bromine atoms, and a double bond between the central carbon atom and the oxygen atom.
 - a. The two C–Br single bonds will comprise a σ -bond, formed by end-to-end overlap between two of the sp^2 orbitals on the carbon and a p orbital on each of the bromine atoms.
 - b. The C=O double bond will comprise a σ -bond, formed by an end-to-end overlap between the remaining sp^2 orbital on the carbon and an sp^2 orbital on the oxygen (The oxygen has three electron-groups around it, and therefore, is also trigonal planar.), plus a π -bond formed from a side-to-side overlap of a p orbital from the carbon atoms and a p orbital from the oxygen atom.

G. **Try these same procedures on the following molecules and polyatomic ions:**

1. ClO_3^-
2. SO_3
3. SO_2
4. SO_4^{2-}
5. SnCl_2
6. NCO^-
7. PF_6^-