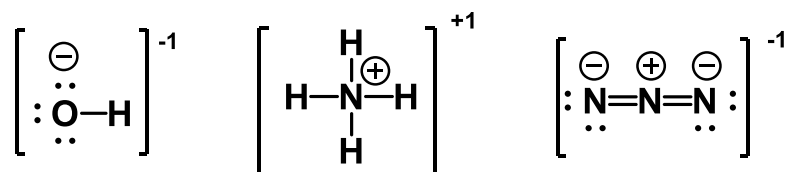
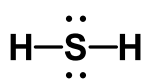


1. Calculate and label the formal charge of each atom in the following structures. Determine the overall charge of each molecule or complex ion if any.

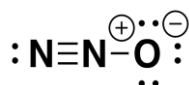


2. Draw the best Lewis structure for the following molecules:

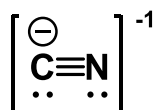
a)



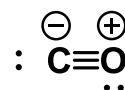
b)



c)



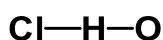
d)



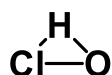
3. Hypochlorous acid has the molecular formula HOCl. There are four possible ways to arrange the atoms in HOCl.

- a) Draw four possible skeletal structures showing atom connectivity below (you do not need to draw full Lewis structures).

Structure 1



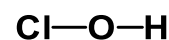
Structure 2



Structure 3



Structure 4



- b) For each of the structures above, briefly explain why it can or cannot be a valid Lewis structure for HOCl.

**Structure 1: Not a good structure because H is the central atom (has more than one bond). Not a valid Lewis structure because octet rule not satisfied for both Cl and O, and duet rule not satisfied for H.**

**Structure 2: Not a valid Lewis structure because it is a three-member ring, with two bonds to H, so duet rule for H not satisfied.**

**Structure 3: Can be a valid Lewis structure because octet rule can be satisfied for O and Cl, and duet rule for H. Not the best structure because formal charges are not minimized when the octet rule is followed.**

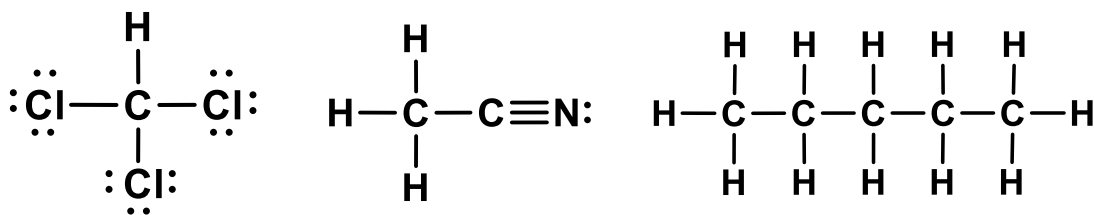
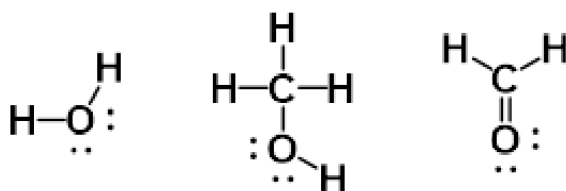
**Structure 4: Is the best Lewis structure because the octet and duet rules can be satisfied, resulting in the minimum charges on all atoms.**

**Remember that for oxyacids, the H atom is bonded to oxygen.**

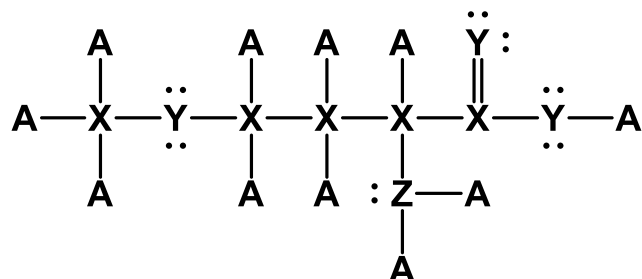
4. Fill in the table with the number of lone pairs and bonds that each element needs in order to have a formal charge of 0.

Element	Lone pairs	Bonds	Formal Charge
C	0	4	0
N	1	3	0
O	2	2	0
F	3	1	0

5. **Good Question.** Draw the best Lewis structure for each of the following common solvents. water ( $\text{H}_2\text{O}$ ), methanol ( $\text{CH}_3\text{OH}$ ), formaldehyde ( $\text{CH}_2\text{O}$ ), chloroform ( $\text{CHCl}_3$ ), acetonitrile ( $\text{CH}_3\text{CN}$ ), pentane ( $\text{C}_5\text{H}_{12}$ ).

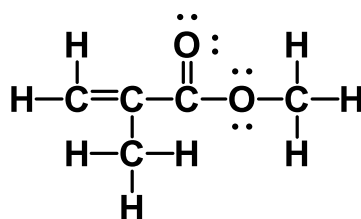


6. **Good question.** A molecule with zero formal charges on all atoms is drawn below. Identify which group of the periodic table each of the elements X, Y, Z, and A, belong to.



**X: Group 14      A: Group 1**  
**Y: Group 16      Z: Group 15**

7. **Good question.** Poly(methyl methacrylate) (PMMA) is a polymer commonly known as acrylic glass and commercially sold under the tradename Plexiglas®. PMMA is synthesized by the polymerization of methyl methacrylate (MMA). The skeletal structure (showing atom connectivity) of MMA is shown below. Draw multiple bonds and lone pairs as necessary to show the best Lewis structure of MMA.

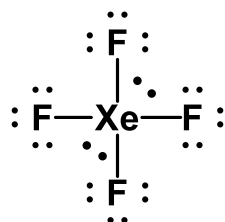


8. Draw the best Lewis structures of (a)  $\text{AlF}_3$  and (b)  $\text{XeF}_4$ :

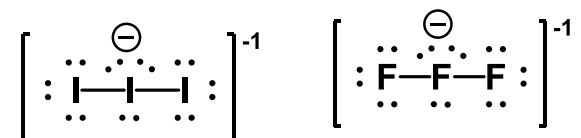
a)



b)

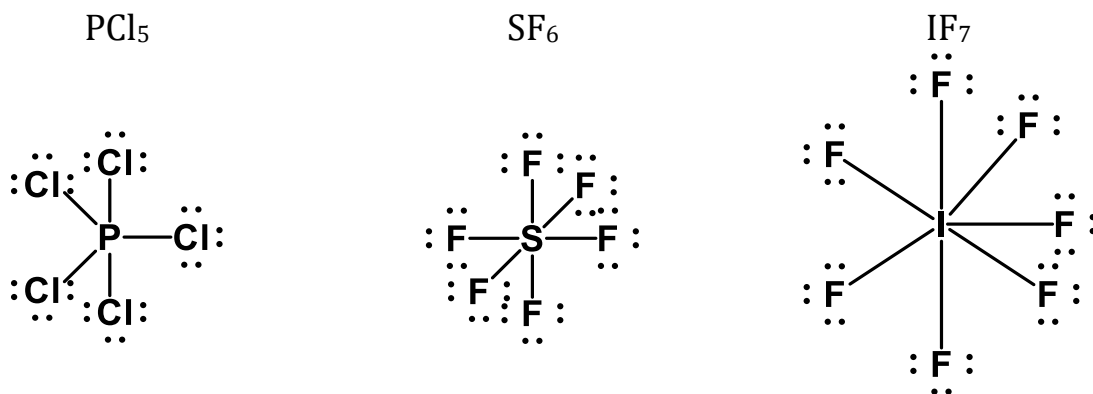
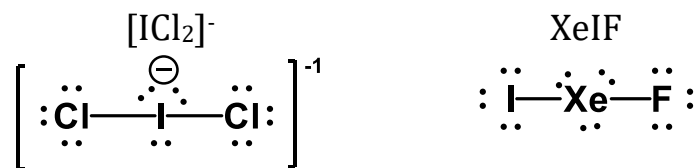


9. Draw the best Lewis structure of  $[I_3]^-$ . Provide a reasonable explanation why  $[F_3]^-$  is not found in nature.

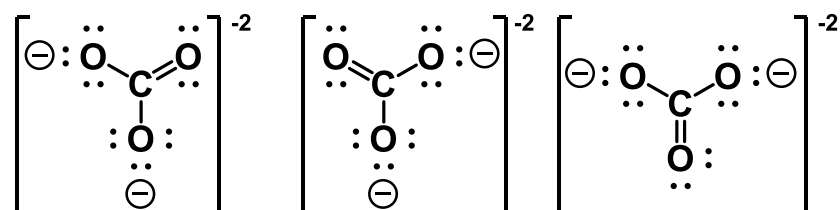


**The analogous structure for  $[F_3]^-$  (shown above) does not occur because fluorine cannot expand its octet so cannot play the role of a central atom.**

10. **Good practice.** Draw the best Lewis structure for:  $[ICl_2]^-$ , XeIF,  $PCl_5$ ,  $SF_6$ ,  $IF_7$ . (You will need to read about hypervalency to answer this question)

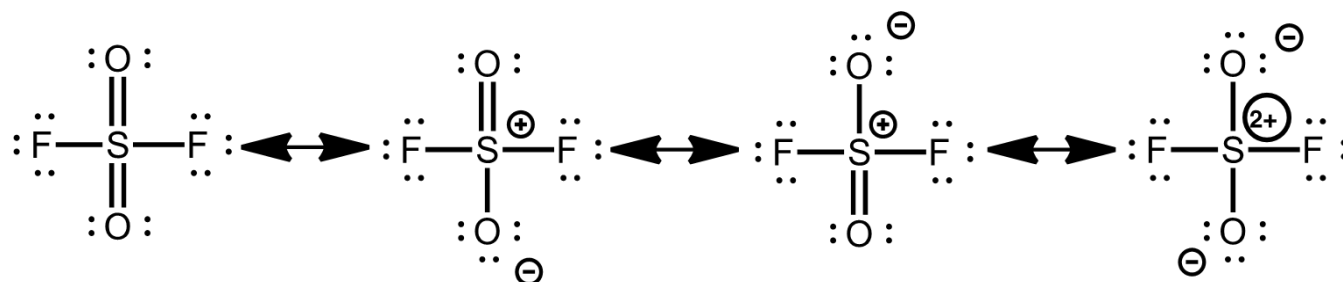


11. Draw ALL chemically reasonable Lewis structures of  $[CO_3]^{2-}$ . Estimate the bond order for each C-O bond.



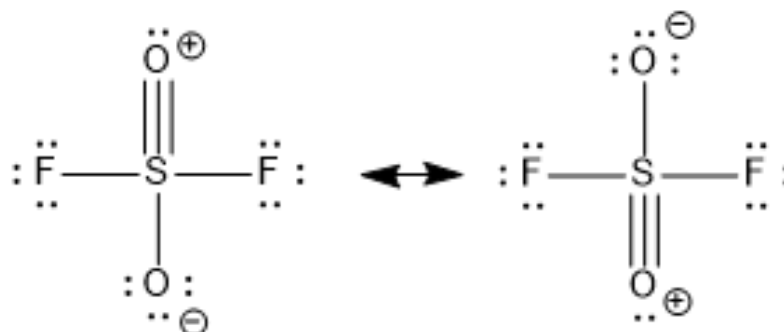
**Because all the resonance structures are equivalent, all the C-O bonds are equivalent and the estimated C-O bond order is an equally weighted average over the three structures, that is  $(2+1+1)/3 = 4/3$ .**

12. Draw ALL chemically reasonable Lewis structures (including resonance structures) of  $\text{SO}_2\text{F}_2$  having S as the central atom. Propose reasons why the linearly-connected structure  $\text{F-O-S-O-F}$  is not found in nature.



**Do NOT make multiple bonds to terminal halogens and do not put negative charges on a central atom if hypervalency is used.**

**The two structures to the right are also valid, in the sense they do not violate any of the Lewis structure rules. However, they are not chemically reasonable. As a first step, one should draw resonance structures obeying the octet rule, such**

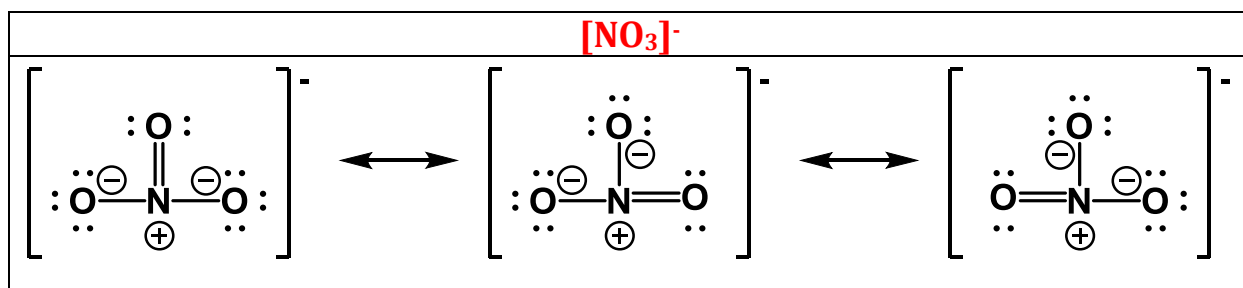
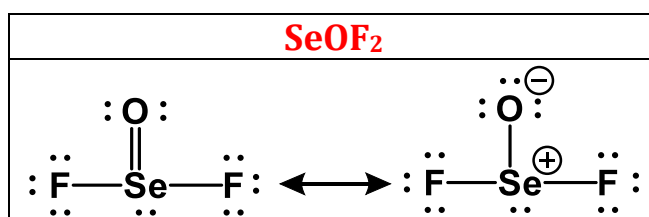


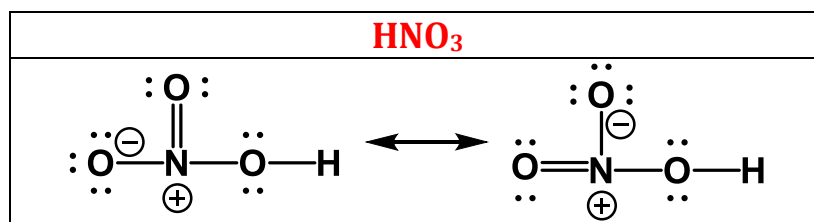
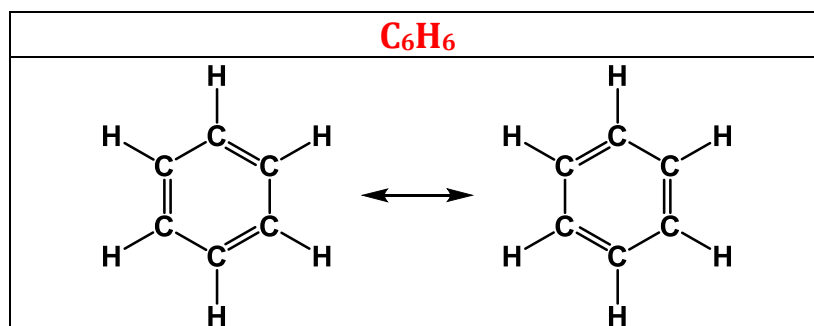
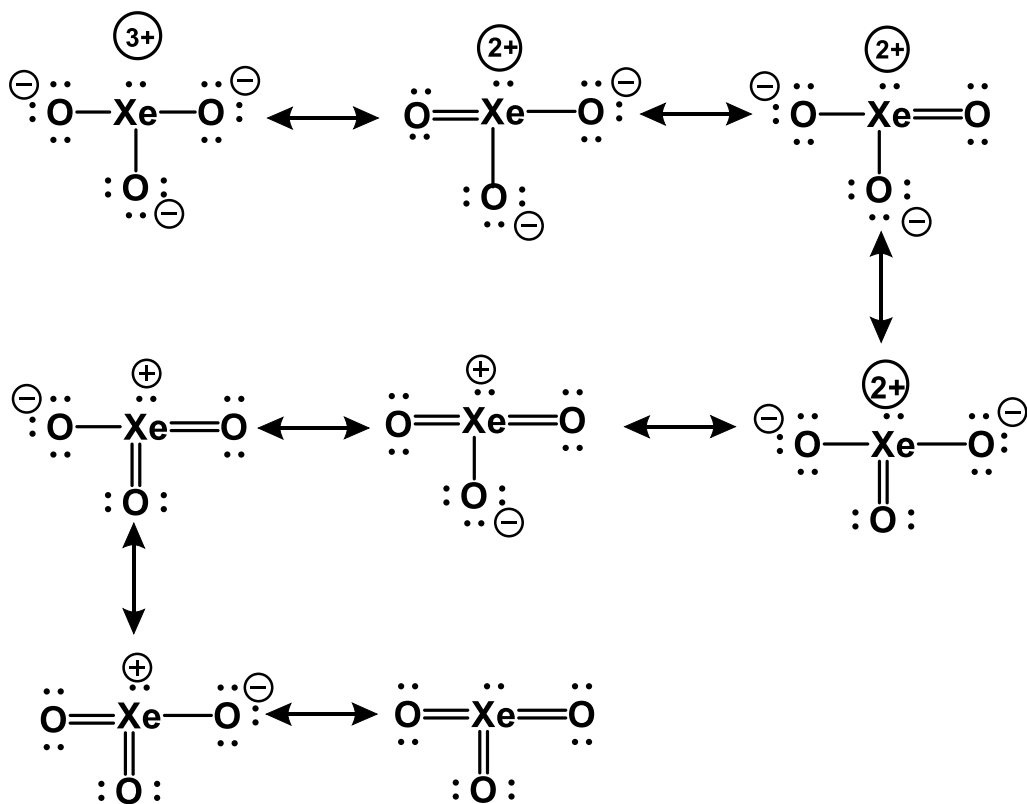
**as the right most one at the very top. Then, let the molecule guide you. In this case, the formal charges are quite large in the octet structure, and it is possible to reduce these by using the allowed hypervalency on S. This produces the two middle resonance structures. The formal charges can be minimized even further by having 6 bonds to the S, as in the left most structure. At this point, the formal charges are as low as they can be so there is no chemically reasonable argument for proceeding further. The two resonance structures containing the SO triple bond also have 6 bonds to S but have introduced a formal charge separation on the oxygens. However, a Lewis structure with this same valency exists with zero formal charges, so it is chemically unreasonable to consider the SO triple-bonded**

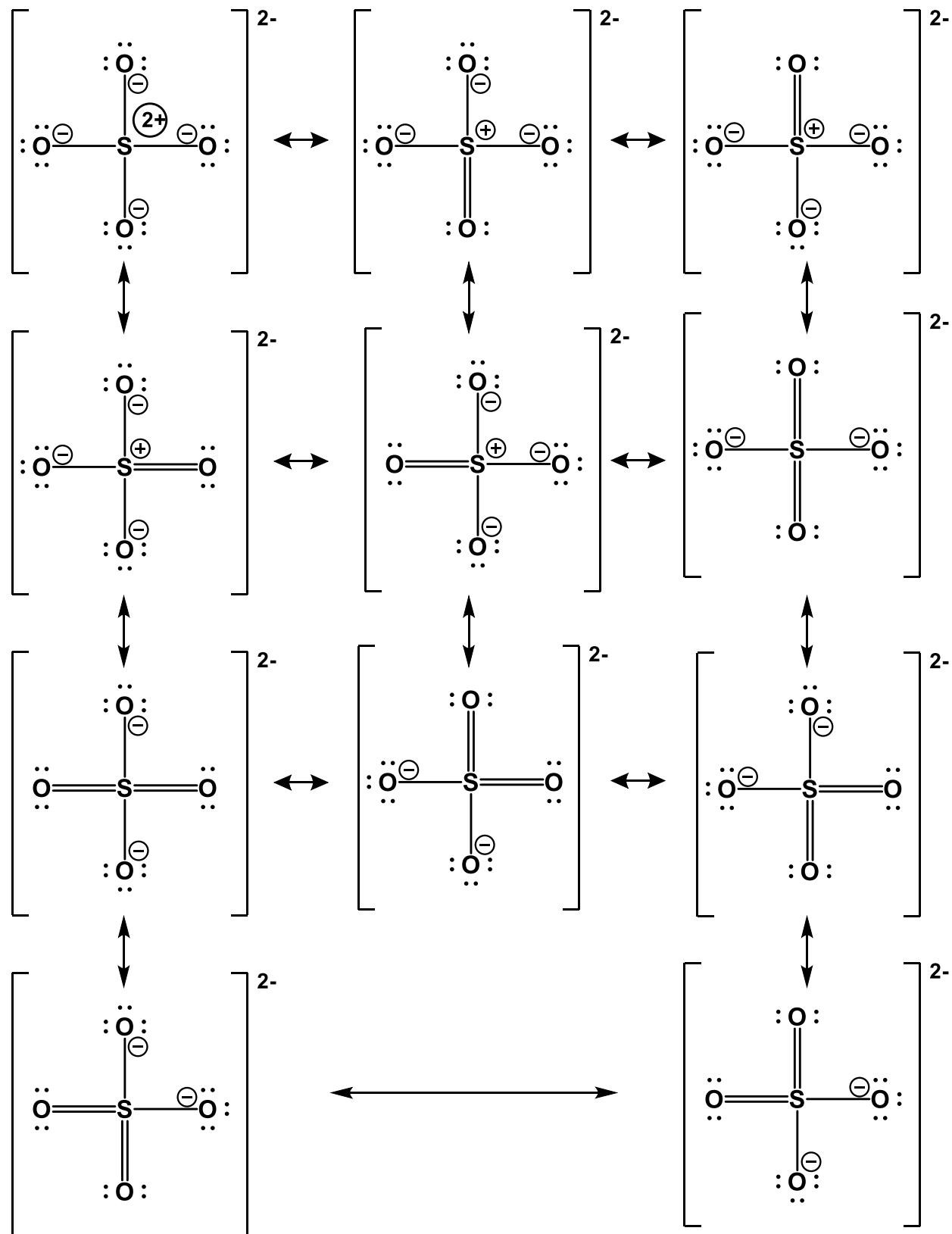
ones, even though they are valid, strictly speaking. This is the distinction between “valid” and “chemically reasonable” Lewis structures.

For the second part of the question, in nature, the structure F-O-S-O-F is not found but H-O-S-O-H is. Both are valid Lewis structures but the absence of the former suggests the reason is due to the fluorine atoms. Think about why the best Lewis structure given above with F bonded to S would be better than the linearly-connected Lewis structure with F bonded to O.

13. Good practice. Draw ALL chemically reasonable Lewis structures (including resonance structures) for:  $[\text{SO}_4]^{2-}$ ,  $\text{XeO}_3$ ,  $\text{SeOF}_2$ ,  $[\text{NO}_3]^-$ ,  $\text{C}_6\text{H}_6$  (draw a ring),  $\text{HNO}_3$ .

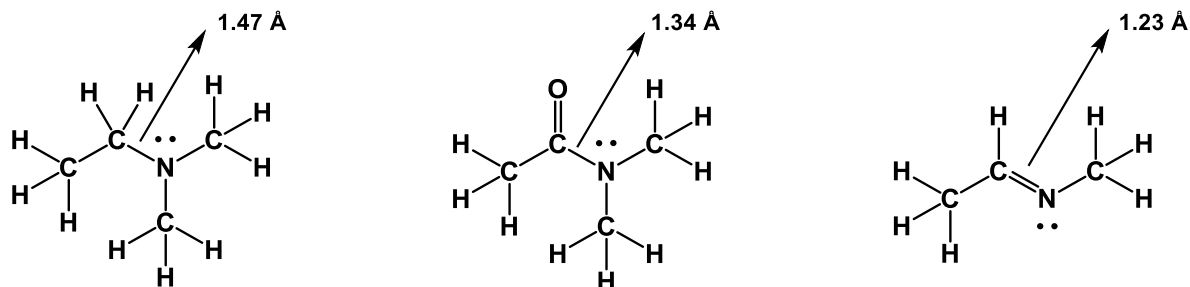


 **$\text{XeO}_3$ :**

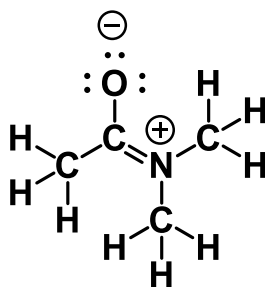




14. **Good question.** The carbon-nitrogen bond length for three organic compounds is shown below. Briefly explain this trend.



The molecule in the middle has the valid resonance structure shown below. The other two molecules do NOT have valid resonance structures. For this reason, the molecule on the left has the lowest C-N bond order (a single bond with bond order 1) and the longest bond; the structure on the right has a bond order of 2 and the shortest bond; and the structure in the middle has a bond order between that of the other two structures because of the contributions of the resonance structure. So, its bond length should also be between these two limits, as the numerical value shows.



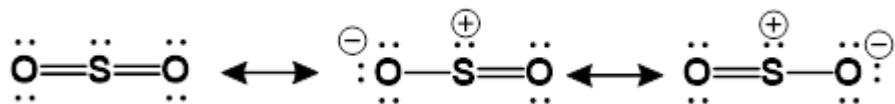
15. **Good practice.** Sulfur has amongst the most diverse chemistry of all of the atoms of the periodic table. For example, it forms a large number of different compounds in the presence of oxygen, including  $\text{SO}_2$ ,  $\text{SO}_3$ ,  $\text{SO}_3^{2-}$  and  $\text{SO}_4^{2-}$ . In each of these molecules, the S-O bond distances are different, as can be seen in the table at right. Provide a *rationale* for the reported bond distances for each of these species.

Use the most stable Lewis structures for each species (shown below and in Question 13 for  $[\text{SO}_4]^{2-}$ ) to estimate bond orders for the S-O bond. For  $[\text{SO}_3]^{2-}$  and  $[\text{SO}_4]^{2-}$ , these correspond to the best equivalent structures having negative formal charges on two oxygen atoms, giving bond order estimates of 1.33 and

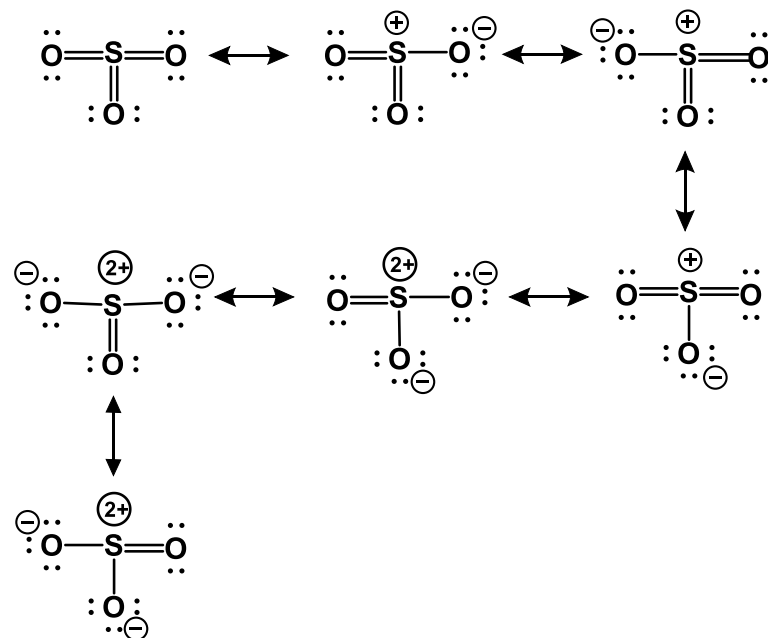
	Bond Order	$r_{\text{SO}}$ (pm)
$\text{SO}_2$	1.66	144
$\text{SO}_3$	1.75	142
$[\text{SO}_3]^{2-}$	1.33	152
$[\text{SO}_4]^{2-}$	1.50	149

**1.5, respectively. For  $\text{SO}_2$  and  $\text{SO}_3$ , the best structures (with all formal charges zero) predict the same bond order of 2 so we need to include the next best structures with +1 on S and -1 on one O to distinguish them. Treating these structures as equivalent (which will slightly underestimate the bond order) gives bond order estimates for  $\text{SO}_2$  and  $\text{SO}_3$  as 1.66 and 1.75, respectively. As the table entries show, as the bond order increases, the bond length decreases, as one would expect.**

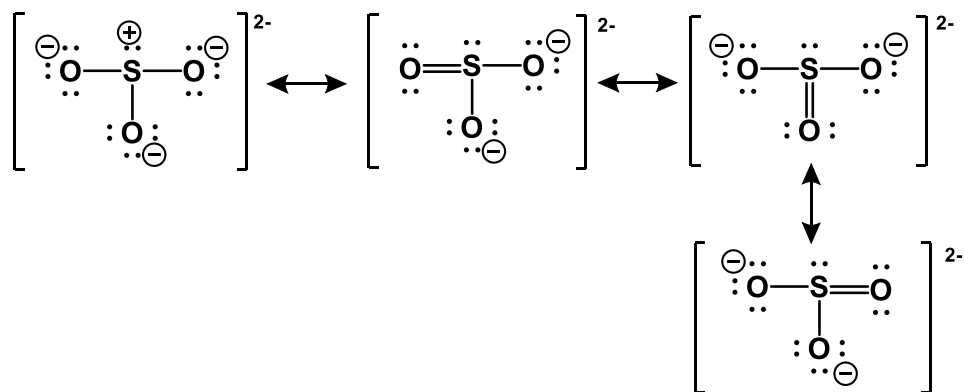
**$\text{SO}_2$ :**



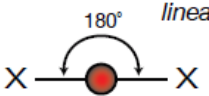
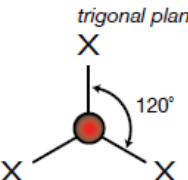
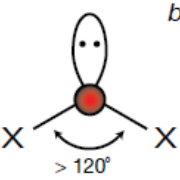
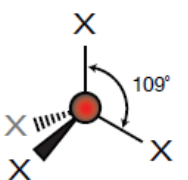
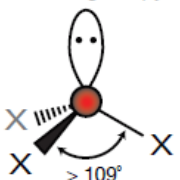
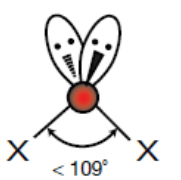
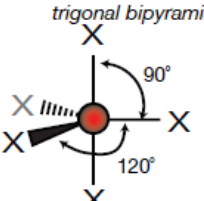
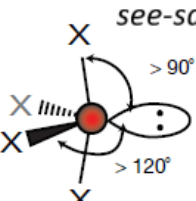
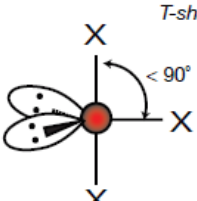
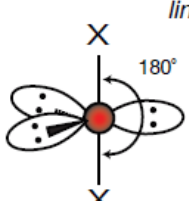
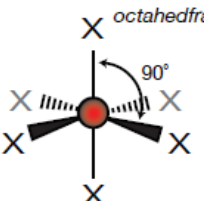
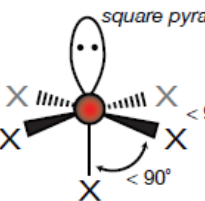
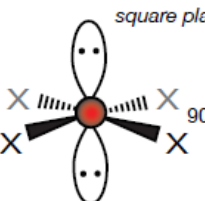
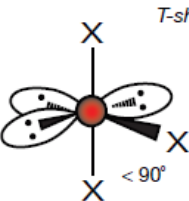
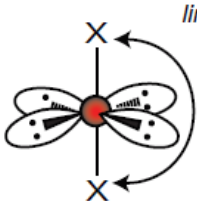
**$\text{SO}_3$ :**



**$[\text{SO}_3]^{2-}$ :**



16. Using <https://phet.colorado.edu/en/simulation/molecule-shapes>, the PhET applet “Molecular Shapes”, complete the table below by drawing perspective diagrams, naming the shapes, and giving the bond angles formed when bonds are replaced with lone pairs in the given parent shapes.

0 lone pairs		1 lone pair		2 lone pairs		3 lone pairs		4 lone pairs	
Number of atoms around the central atom (steric number)	2								
	3								
	4								
	5								
	6								

17. Fill in each of the blanks in the table below. For the Lewis structures, write any non-zero formal charges on the appropriate atoms, show all lone pairs of electrons as pairs of dots and all bond pairs as lines.

Molecule	Best Lewis structure	Parent shape	Molecular shape	Perspective diagram	Polar? (Yes/No)
$\text{AlCl}_3$		Trigonal planar	Trigonal planar		N
$\text{PH}_3$		Tetrahedral	Trigonal pyramidal		Y
$\text{H}_2\text{O}$		Tetrahedral	Bent		Y
$\text{SOF}_2$		Tetrahedral	Trigonal pyramidal		Y

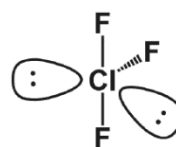
18. **Good practice.** Complete the table below:

Molecule	Best Lewis structure	Parent shape	Molecular shape	Perspective diagram	Polar (Yes/No)
$\text{CBr}_2\text{F}_2$		<b>Tetrahedral</b>	<b>Tetrahedral</b>		<b>Y</b>
$[\text{I}_3]^-$		<b>Trigonal bipyramidal</b>	<b>Linear</b>		<b>N</b>
$\text{C}_2\text{F}_4$		<b>Trigonal planar</b>	<b>Trigonal planar</b>		<b>N</b>
$\text{XeF}_4$		<b>Octahedral</b>	<b>Square planar</b>	<p>Preferred</p> <p>Acceptable</p>	<b>N</b>
$\text{XeOF}_4$		<b>Octahedral</b>	<b>Square pyramidal</b>		<b>Y</b>

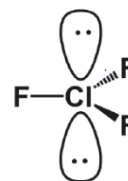
19.  $\text{ClF}_3$  has a trigonal bipyramidal parent shape with two lone pairs on the central atom. As such, it can take have two possible molecular shapes: T-shape or trigonal planar (see below).

- a) Determine the number of  $90^\circ$  LP-LP, LP-BP, and BP-BP interactions in each of these geometries. Write your answers in the table below.

	T-shape	Trigonal planar
LP – LP	0	0
LP – BP	4	6
BP – BP	2	0



T-shape



Trigonal planar

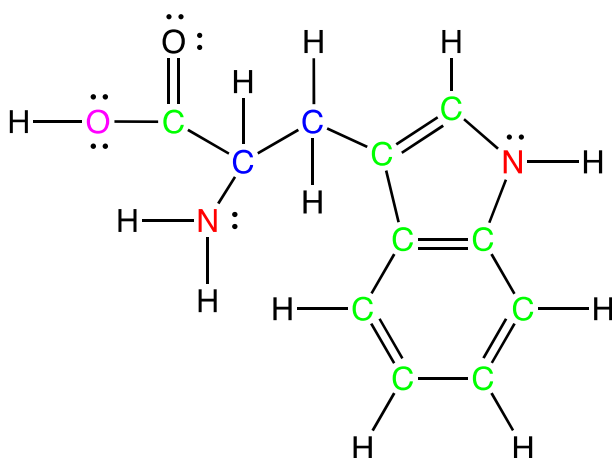
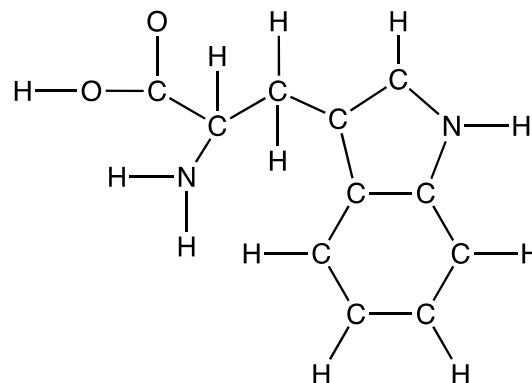
- b) Based on your answers to a., which molecular geometry is  $\text{ClF}_3$  more likely to exhibit? Briefly explain your answer.

**A molecule will take the shape that minimizes the number of smallest angle LP-LP interactions. If those are the same, LP-BP interactions must be minimized before minimizing BP-BP interactions. In this case, the smallest angle for LP-LP, LP-BP, and BP-BP interactions is  $90^\circ$  so, the question is explicitly telling us to look at  $90^\circ$ . In some cases, you may need to determine the smallest angle interactions by examining a diagram, like that above.**

**As the table shows, there are 0 LP-LP interactions in both geometries. Therefore these will NOT impact the shape of the molecule.  $90^\circ$  LP-BP interactions are minimized in the T-shape (4 vs. 6). Therefore the molecule must exhibit a T-shape. Note that once LP-BP interactions are minimized, one does NOT need to consider BP-BP interactions, because they are less important. There is a hierarchy of interactions with LP-LP ones being the most important to consider, and BP-BP ones the least important.**

20. **Good question.** The skeletal structure (showing atom connectivity) of tryptophan, an essential amino acid, is shown to the right. The formal charge on all atoms of the best Lewis structure of tryptophan is zero.

- Complete the skeletal structure so that it is a valid Lewis structure
- Identify all atoms with a trigonal pyramidal molecular shape
- Identify all atoms with a trigonal planar molecular shape



**Trigonal pyramidal centres labelled in red.**

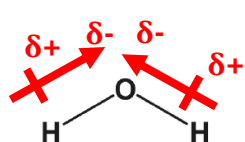
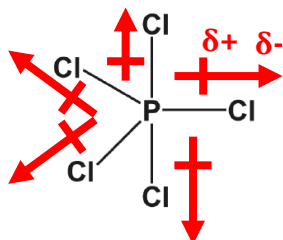
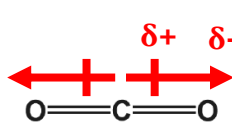
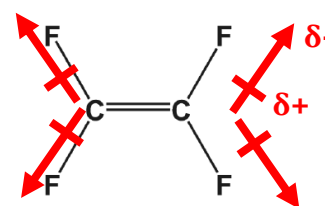
**Trigonal planar centres labelled in green.**

**Tetrahedral centres labeled in blue**

**Bent centres labeled in pink**

**Remember that VSEPR parent shapes and molecular shapes are determined using the best Lewis structure (i.e. the structure with fewest formal charges).**

21. Add arrows to show bond dipoles for the following polar covalently bonded compounds. Add  $\delta+$  and  $\delta-$  to the following structures. Lone pairs are NOT shown. Determine which molecules are polar and which are non-polar.

**Polar****Non-polar****Non-polar****Non-polar**

**$\delta+$  and  $\delta-$  labels are only placed in one bond for clarity.**

22. **Good practice.** A molecule with the formula  $AX_4$  in which A is a central atom and X is a terminal halogen has 34 valence electrons. Is the molecule polar? Briefly explain your answer with a diagram.

**A molecule  $AX_4$  with a terminal halogen has the structure below. Terminal halogens are single bonded to the central atom and as such have three lone pairs each. The structure below to the far left has 32 electrons. The question states the structure has 34 electrons. We will add 2 more electrons to the central atom to account for all valence electrons (middle structure). The VSEPR shape of this molecule is shown below to the far right. This molecule exhibits a see-saw shape which is polar.**

<b>32 electrons</b>	<b>34 electrons</b>	<b>VSEPR shape</b>