

Chapter 29

SHAPE, Part 2 and POLARITY

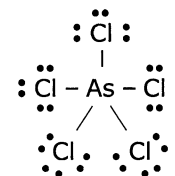
©2004, 2008, 2011, 2022 Mark E. Noble

We continue.

29.1 More examples

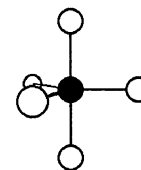
Example 7. Arsenic pentachloride.

► Step 1. Lewis structure.

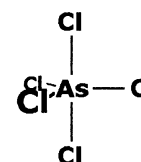


► Step 2. The arsenic has five bonded atoms and zero LPs. The sum is five. The VSEPR classification is AX_5 .

► Step 3. For a sum of five, the orientation of least repulsion is trigonal bipyramidal. The angles are 90° , 120° and 180° .



► Step 4. The chlorine atoms are located at all five TBP locations. This gives the final shape as TBP. The Cl-As-Cl bond angles are 90° , 120° and 180° .

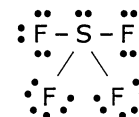


Since there are no lone pairs on arsenic, the shape is the same as its orientation of least repulsion.

Due to the peculiarities of TBP orientation, new considerations arise when lone pairs are present on the central atom. These are a bit more vexatious to the spirit. We see this in the very next Example.

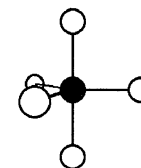
Example 8. Sulfur tetrafluoride.

► Step 1. Lewis structure.

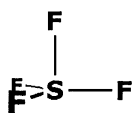


► Step 2. Sulfur has four atoms attached to it and it has one LP. The sum is five. This gives the VSEPR classification AX_4E .

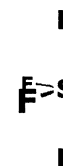
► Step 3. The orientation of least repulsion is TBP.



► Step 4. Fluorine atoms occupy four of the TBP positions, while the fifth position is a lone pair. Now we have a problem.



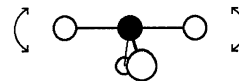
The problem arises because TBP has inequivalent axial and equatorial positions. Since the lone pair is the oddball here, let's focus on that: will the lone pair be axial or will it be equatorial? If the LP is axial, then we get the shape on the left; if the LP is equatorial, then we get the shape on the right. They're different. What's the answer? Well, we need a bit more about repulsions right now.



Everything we've done so far was based on all repulsions being equal. In other words, all lone pairs and all bond pairs are equally repulsive. But that's simply not true: lone pairs are much more repulsive than bond pairs. Why? Lone pairs are attached to one atom only. Bond pairs connect two atoms; both

ends of the bond orbital are attracted to nuclei with their positive charges. This interaction keeps the bonding orbital more compact (less repulsive) than a lone pair orbital. Since LP orbitals are more repulsive, lone pairs need more room around an atom than do bond pairs. Now let's apply this to the tbp orientation in the present Example. Although it may not be obvious, it turns out that equatorial positions have a bit more room than axial positions when it comes to accommodating repulsions. This leads us to the answer for SF_4 : the much-more-repulsive LP will take one of the more-accommodating equatorial positions. This gives the shape on the right above.

The name given to this shape can be seen by laying the shape sideways. Now imagine rocking the molecule: this motion is related to that of a seesaw (teeter-totter), and that is the name of the shape, "seesaw". We say that sulfur tetrafluoride is seesaw shape.



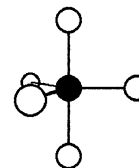
This was our first complication for tbp OLR. Keep in mind that equatorial positions will accommodate repulsions better than axial positions. We'll need this for two more shapes.

.....
Example 9. Chlorine trifluoride.

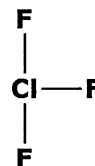
► Step 1. Lewis structure. You do this one.

► Step 2. When you do the Lewis structure, you should see that the VSEPR classification is AX_3E_2 . The sum is five.

► Step 3. The sum of five leads again to tbp orientation.

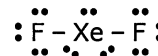


► Step 4. Of the five tbp positions, three are fluorine atoms and two are lone pairs. Both LPs will be equatorial. That leaves one equatorial spot available for one F, while the other two F's will be axial. This gives the shape shown on the right: it's the capital letter 'T', drawn sideways. This shape is called "T-shaped".



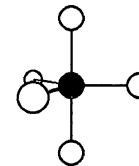
.....
Example 10. Xenon difluoride, XeF_2 .

► Step 1. Lewis structure.

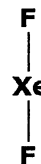


► Step 2. The sum is five; the VSEPR classification is AX_2E_3 .

► Step 3. Again, this calls for tbp orientation.



► Step 4. Here, all three equatorial positions are taken by lone pairs. That leaves the two axial positions for the two fluorines. Since these are directly opposite each other at 180° , the shape is linear.

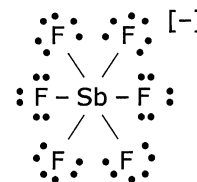


This is our second example with linear shape. The first was Example 1, BeH_2 , in Chapter 28. That one was AX_2 classification, while this one is AX_2E_3 . All linears have 180° bond angles so the F-Xe-F bond angle is 180° , as was true for the bond angle in BeH_2 .

This concludes the shapes derived from tbp orientation. Let's move on to shapes derived from octahedral OLR.

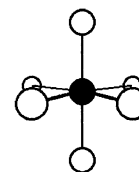
Example 11. Polyatomic anion: SbF_6^- .

► Step 1. Lewis structure.

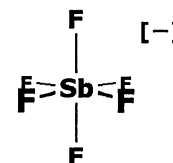


► Step 2. The central antimony has six atoms bonded to it and it has zero LPs. The sum is six. The VSEPR classification is AX_6 .

► Step 3. For a sum of six, the orientation of least repulsion is octahedral. The angles are 90° and 180° .



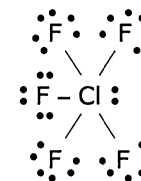
► Step 4. The six fluorine atoms are positioned at all six of the octahedral locations. The shape is octahedral. The F-Sb-F bond angles are 90° and 180° .



As we have seen before, when the central atom has no lone pairs, then its shape is the same as its OLR.

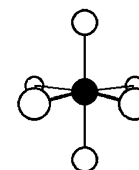
Example 12. Chlorine pentafluoride.

► Step 1. Lewis structure.

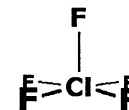


► Step 2. Chlorine is bonded to five atoms and it has one LP. The sum is six, and the VSEPR classification is AX_5E .

► Step 3. The orientation of least repulsion is octahedral.



► Step 4. Fluorine atoms occupy five of the six octahedral locations; the sixth position is a lone pair. The shape is another pyramid, but now the pyramid has a square as a base. The term for this shape is "square pyramidal".



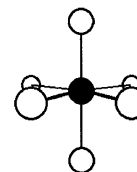
Since all positions of an octahedron are equivalent, it does not matter where you locate the LP for ClF_5 . You will get the same shape regardless, although it would point in a different direction.

Example 13. IF_4^- . We've been talking about this ion since Chapter 26.

► Step 1. Lewis structure. We did this in Chapter 26; go back and look.

► Step 2. We did this in Chapter 28: the sum is six and it's AX_4E_2 .

► Step 3. For a sum of six, the orientation of least repulsion is octahedral.



► Step 4. We have four fluorines and two LPs to accommodate. There is now a new twist which we must consider.

As shown in Example 12, one LP can be drawn anywhere in octahedral orientation. We'll place the first LP in the bottom here, as for ClF_5 above. Now, the second LP position does matter: it can be positioned next to the first (as shown at left) or it can be positioned opposite the first (as shown at right). Which is it? The answer lies again in the relative repulsions. Since lone pairs are more repulsive than bond pairs, the two LPs will want to be furthest from each other. This means that they want to be on opposite sides from each other and this means that you get the shape which is shown above at right. In this shape, all atoms lie in a plane and this plane makes up a square; the shape is called "square planar". In order to see this better, I've drawn it again at right with the plane flipped for better clarity.

That ends it: thirteen variations on shape. I said "variations on shape". There are only eleven different shapes but there are two variations for linear (AX_2 and AX_2E_3) and there are two variations for bent (AX_2E and AX_2E_2). It's important that you work with all of the shapes and try to get comfortable with them. Yes, there are a lot of them but don't blame me; Nature made it that way.

Let's summarize all of these shapes so far.

29.2 Three summaries

We shall summarize these in three ways. Actually, you're going to do the summaries. I'm leaving blanks. The whole idea of this is to give you more practice with the system. Have your model kits handy, or at least be ready to sketch things out.

The summaries will just use VSEPR classifications and they will avoid actual compound formulas. Right now, the focus is on shape so I don't want to slow this down with Lewis structures for compounds.

• FIRST SUMMARY

This First Summary follows exactly the sequence of all Examples 1 - 13. Fill in the blanks. For the given classification, enter the sum of lone pairs plus bonded atoms. For this sum, enter the correct orientation of least repulsion. Then, based only on atom positions, select the correct shape. Try to do this without looking anything up. If you are having trouble, then go back to the Examples. The answers are in Examples 1 - 13, in that order.

	Classification	Sum	OLR	Shape
1.	AX_2	_____	_____	_____
2.	AX_3	_____	_____	_____
3.	AX_2E	_____	_____	_____
4.	AX_4	_____	_____	_____
5.	AX_3E	_____	_____	_____
6.	AX_2E_2	_____	_____	_____
7.	AX_5	_____	_____	_____

8.	AX_4E	_____	_____	_____
9.	AX_3E_2	_____	_____	_____
10.	AX_2E_3	_____	_____	_____
11.	AX_6	_____	_____	_____
12.	AX_5E	_____	_____	_____
13.	AX_4E_2	_____	_____	_____

Although that may be tedious, that Summary is the easy one. Let's go to the next.

• SECOND SUMMARY

This Second Summary is arranged by the number of bonded atoms and then by the number of lone pairs on the central atom. This is a different sequence from the one above. Again, you fill in the blanks. For the given number of bonded atoms and the given number of lone pairs, enter the sum. Then enter the correct orientation of least repulsion and then shape. Try to do this without looking at the Examples or the First Summary. When you are done or if you need help, then look back to the Examples or to the First Summary. All the answers are there, but things are now in a different order.

Bonded Atoms	Lone Pairs	Sum	OLR	Shape
2	0	_____	_____	_____
2	1	_____	_____	_____
2	2	_____	_____	_____
2	3	_____	_____	_____
3	0	_____	_____	_____
3	1	_____	_____	_____
3	2	_____	_____	_____
4	0	_____	_____	_____
4	1	_____	_____	_____
4	2	_____	_____	_____
5	0	_____	_____	_____
5	1	_____	_____	_____
6	0	_____	_____	_____

• THIRD SUMMARY

This one is completely backwards from the first two: it starts with shape. Furthermore, there is no set order to this sequence; I just jumbled them up. For each shape, enter the orientation from which it is derived. Then enter the number of bonded atoms and then the number of lone pairs. As before, the answers are in prior Examples and Summaries; go look there for checking your answers or for help.

Shape	OLR	Bonded Atoms	Lone Pairs
tetrahedral	_____	_____	_____
square pyramidal	_____	_____	_____
trigonal planar	_____	_____	_____
linear (one variation)	_____	_____	_____
linear (other variation)	_____	_____	_____
octahedral	_____	_____	_____
trigonal bipyramidal	_____	_____	_____
bent (one variation)	_____	_____	_____
bent (other variation)	_____	_____	_____
T-shaped	_____	_____	_____
seesaw	_____	_____	_____
trigonal pyramidal	_____	_____	_____
square planar	_____	_____	_____

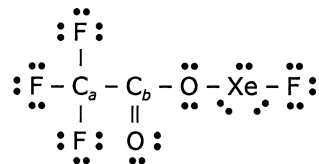
You can use these Summaries for quick reference.

29.3 More than one central atom

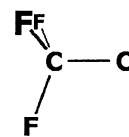
All examples so far had only one central atom. VSEPR can also handle polyatomics with more than one central atom. In these cases, you treat each central atom separately: just go through the steps, one central atom at a time. You determine the shape for each central atom as you go.

Let's do an example which is a bit more involved than the ones above: $\text{CF}_3\text{CO}_2\text{XeF}$. No, this is not your typical, everyday compound but I chose it because it has atoms of different shapes and it will illustrate how these are strung together.

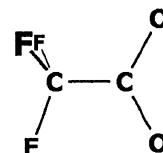
I give the Lewis structure at right. There are four central atoms: both C's, one O and the Xe. All fluorines are terminal and so is the other oxygen. I've labeled the C's in the Lewis structure for easy reference below. Go through the molecule, one central atom at a time. We'll start at the left of the molecule with the first central atom, C_a .



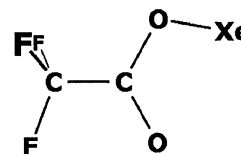
► C_a : From the Lewis structure, we see that this carbon has four atoms attached and it has zero lone pairs. The classification is AX_4 . The sum is four, so the orientation is tetrahedral. There are no lone pairs on C_a , so the shape is tetrahedral. Draw in this atom, along with those atoms which are bonded to it (three F's and C_b).



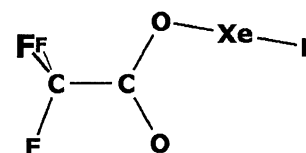
► C_b : From Lewis, we see that this carbon has three attached atoms and zero lone pairs. It is AX_3 . The sum is three, and the orientation is therefore trigonal planar. All three positions are occupied by atoms and it has no lone pairs; the shape for C_b is trigonal planar. Draw in the other atoms which are bonded to C_b ; both O's and C_a are all at 120° to each other.



► O (central, not terminal): From Lewis, this oxygen has two attached atoms and it has two lone pairs, so it's AX_2E_2 . The sum is four. For a sum of four, the OLR is tetrahedral. Two of the tetrahedral positions are bonded atoms (C_b and Xe); the shape is bent. Draw in the Xe on O so that it is bonded at 109.5° relative to C_b .



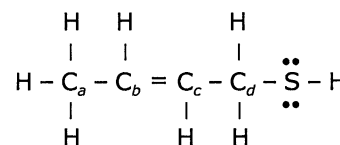
► Xe: From Lewis, this atom has two atoms attached to it and it has three lone pairs. It is AX_2E_3 . The sum is five, so the orientation is tbp. The LPs take all three equatorial positions of the tbp; this leaves the bonded atoms at the two axial positions. The shape for Xe is linear: draw in the bonded F, across (180°) from the oxygen.



That's all there is to it. You do one central atom at a time, constructing the molecule as you go.

Your turn.

Here's a real stinker: it's one of the nasty smell components in skunk spray. You do the shapes for the five central atoms. Just fill in the shapes below. You can sketch it out if you want in the space provided.



C_a _____
 C_b _____
 C_c _____
 C_d _____
 S _____

I'll give one clue: for the five central atoms, three different shapes are involved.

29.4 Another angle on VSEPR

Everything which we've completed so far is basic VSEPR. Like so many other systems, there are also refinements to VSEPR which can run into more and more details. I don't want all of those but I will talk about one of them.

Let's go back to bond angles. We've discussed the various angles associated with the five orientations of least repulsion. Here's the summary from the last Chapter again.

SUM ($n + m$)	ORIENTATION OF LEAST REPULSION	ANGLES
2	linear	180°
3	trigonal planar	120°
4	tetrahedral	109.5°
5	trigonal bipyramidal	$90^\circ, 120^\circ, 180^\circ$
6	octahedral	$90^\circ, 180^\circ$

A bit later after this summary in Chapter 28, I said

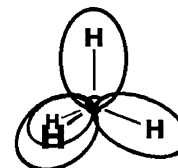
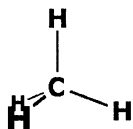
“ The angles for the OLRs, as given above, are the starting points for evaluating bond angles by VSEPR. The actual bond angles in actual compounds may be different from those but the above angles still provide a starting point. We shall see later why those differences arise. But that's later. ”

Later is now.

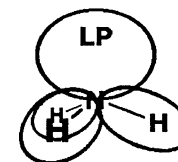
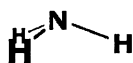
In many cases, an actual polyatomic unit will have bond angles which match the above angles but, in many other cases, there will be differences from those angles. The reason for this goes back to the fact that not all repulsions are equal. Lone pairs are more repulsive than bond pairs, and we saw the effects of this for various shapes. Now, we shall see the effects on bond angles.

Before we go there, let me point out that you will indeed get the above angles whenever all repulsions are equal at equivalent positions around the central atom. This occurred in the prior VSEPR Examples of BeH_2 (Example 1), BH_3 (Example 2), SiCl_4 (Example 4), AsCl_5 (Example 7) and SbF_6^- (Example 11). Whenever you have a single central atom with no lone pairs and all terminal atoms are identical, you will have equal repulsions and you will get the ideal OLR angles above. This is the easy part.

If the central atom has one or more lone pairs, then the LPs can cause some angles to bend. In these cases, the bond orbitals get scrunched closer together by the LP orbitals, resulting in bond angles which are less than the ideal OLR angles. Let's compare two simple examples for illustration: methane, CH_4 , and ammonia, NH_3 . As noted in Chapter 28, CH_4 is AX_4 with tetrahedral OLR and tetrahedral shape (at left). The repulsions in CH_4 are due to four identical C-H bond orbitals (at right). Since identical, all repulsions are equal; the ideal H-C-H bond angles of 109.5° are obtained.



Now consider NH_3 : it is AX_3E with tetrahedral OLR but its shape is trigonal pyramidal due to the lone pair (below left). As drawn below at right, the lone pair orbital exerts its more repulsive influence and bears down on the bond orbitals. As a result, the bond orbitals get scrunched a bit closer together. This compresses the H-N-H angle to some value less than 109.5° . What's the actual value? We can't tell from this much by itself. All we can say is that we expect it to be less than 109.5° . The bond angles have been determined experimentally: each angle is 108° , consistent with the expectation.



In most cases, lone pairs on a central atom will cause bond angles to be less than the ideal OLR values. There are only two cases where this doesn't happen: AX_2E_3 (linear) and AX_4E_2 (square planar). See if you can figure out why.

We can summarize all of this into three statements. These statements assume that there is only one central atom in the polyatomic unit and that all terminal atoms X are identical.

- Every molecule of type AX_n (no LPs on A) will have bond angles equal to the ideal OLR angles.
- Every molecule of type AX_2E_3 and AX_4E_2 will have bond angles equal to the ideal OLR angles.
- Everything else will have bond angles less than the ideal OLR angles.

It is important to note that this discussion is only about angles. The overall shape remains the same.

Notice that I keep referring to identical terminal atoms. In other refinements to VSEPR, you can get into angle changes due to different atoms and angle changes due to different bond orders. We won't go into those here. I will, however, add this note at this time: there are also other factors which enter into this bond angle business but these arise from the imperfections of VSEPR itself. VSEPR is very good but it's not perfect. In many cases, VSEPR does not give the correct bond angles. Much of the reason for this is that VSEPR does not take into account the different kinds of orbitals that make up the polyatomic unit. We will see these orbitals in Chapter 30 and 31. Although the bond angles may not be right, VSEPR still gives the correct shape in the majority of cases, and this much is extremely important.

This ends our discussion for VSEPR. We will next go into one very important application of VSEPR: the determination of molecular polarity.

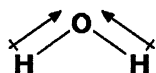
29.5 Molecular polarity

Now we can determine the overall polarity of a molecule. Ultimately, molecular polarity results from the interplay of various influences on charge distribution within a molecule. These influences can include electronegativities, shape, formal charges, bond and lone pair orbitals, etc. For our purposes here, we will keep things simple and only work with the first two: electronegativities and shape. These two aspects

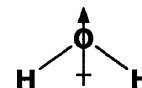
are important to all molecular polarities; the others don't always come into play although I will mention two interesting exceptions to this at the end of this section. We did electronegativities in Chapter 25 and their impact on bond polarity and we have now completed shape with VSEPR.

Ever since Chapter 10, we have used HF as a simple example of a polar molecule. That was easy because HF is diatomic. The molecular polarity of a diatomic is simple: its molecular polarity follows its bond polarity and we derive that from the relative electronegativities of the atoms involved. Shape does not enter into the picture for a diatomic. Go back to the "HF flag" in Chapter 10 and look at the illustrations and discussion there. We didn't do electronegativity at the time.

For molecules with three or more atoms, we must consider all the bond polarities in the various directions according to the shape of the molecule. We referred to this when we first talked about the polarity of water, also in Chapter 10. Go back to the "H₂O flag" in Chapter 10 and look at that part also. We now know that water has two O-H polar bonds due to the electronegativities of O and H. We also know that H₂O is AX₂E₂ and that the shape is bent; the H-O-H bond angle is derived from 109.5°. (Due to the lone pairs, we expect the bond angle to be less than this; experimentally, the angle is 104.5°.)

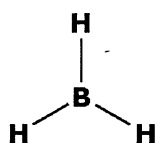
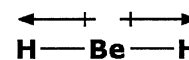


Let's consider two bond polarities in bent shape (at left); it is their sum which determines the overall molecular polarity (at right). The side of the molecule with the oxygen is somewhat negative, while the side with the two hydrogens is somewhat positive.



Water is a simple case and hopefully you can see how the two bond polarities add to give the overall molecular polarity. Unfortunately, this kind of approach can get difficult for more complicated cases. The problem is that this stuff is best handled by vector algebra, since all of these arrow gizmos are vectors. If you are familiar with vector math, then we are taking resultants of the bond polarities to get the molecular polarity. If you are not into vector math, then don't panic; we are not going into the mathematical details.

There are two ways to approach this qualitatively. Imagine each arrow for bond polarity as a push in the arrow direction. The question which you must consider is this: do the pushes of the separate arrows cancel each other out or not? In the case of H₂O, the two bond polarities do not cancel out exactly, so the molecule is polar overall. If, however, the pushes do cancel out exactly, then the molecule is nonpolar. To show that, let's go back to our simplest example of shape, BeH₂. This was linear shape. The polarity of each Be-H bond is Be(δ⁺)-H(δ⁻). I sketch these at right. Now you have equal but opposite pushes away from the central atom. Since they are equal and opposite, they cancel each other completely. Since they cancel each other completely, BeH₂ has no molecular polarity. Although the bonds are polar, the overall molecule is nonpolar.

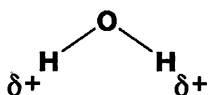


Unfortunately, beyond linear shape, this analysis gets troublesome. Let's do BH₃. The polarity of each B-H bond is B(δ⁺)-H(δ⁻). You can draw the bond polarity arrows into the diagram at left. Now, try to figure out if they cancel exactly or not. What do you think? This one is not obvious at all, but all three bond polarities do cancel each other out completely. This means that BH₃ is nonpolar.

Already this approach is getting a bit difficult. Let me bring in the other non-math approach. This one assesses molecular polarity based on the partial charges of terminal atoms only.

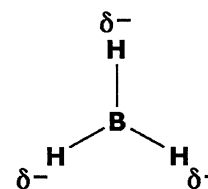
For any molecule with one and only one central atom, consider the distributions of the partial charges of the terminal atoms. For this analysis, you do not need to look at the central atom's partial charge so don't bother with that one. Just look at the partial charges on the terminal atoms which are due to bond polarity. If the partial charges are equal and evenly distributed around the central atom, then the molecule is nonpolar. If the partial charges are not equal and evenly distributed around the central atom, then they will not cancel and the molecule is polar.

Using this approach, BeH₂ is shown at right with the partial charges shown for the terminal atoms only. The δ⁻ partial charges on the two hydrogens are equal and they are evenly distributed around the central atom. Therefore, nonpolar.



H₂O is shown at left with the terminal atom partial charges only. The δ⁺ partial charges for H are all on one side (bottom side) of the central O and there are none on the other side (top side). Therefore, these are not evenly distributed; the molecule is polar.

Now consider BH_3 at right with the terminal atom partial charges only. These are equal and evenly distributed around the central atom. Therefore, the molecule is nonpolar.



Again, we are only looking for an equal and even distribution of partial charges on terminal atoms only. We are leaving out the central atom's partial charge. Ultimately, ALL partial charges (terminal and central) will cancel out in a neutral molecule but that is separate from the current analysis.

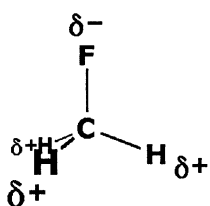
Both of the above approaches are pictorial for assessing molecular polarity. There's also a memorization method, if you want to do that instead. This method applies when there is only one central atom in the polyatomic unit and all terminal atoms X are identical.

- Every molecule of type AX_n (no LPs on A) is nonpolar.
- Every molecule of type AX_2E_3 and AX_4E_2 is nonpolar.
- Everything else is polar.

As you may notice, these statements are broken down exactly as for bond angles above and they have the same conditions as underlined. Why do the polarity and bond angle relationships break down exactly the same? It's got to do with symmetry and that would take a bit more math than we need to get into. We'll stick with these statements as presented.

If there is more than one central atom, then the above methods won't work. You have to look at all atoms of the molecule as a whole and these cases can get complicated. We won't do those here. We'll do some beginning in Chapter 37 when we hit more applications of polarity. We have enough for the here and now.

So far, all examples have involved identical terminal atoms. If you have one central atom but the terminal atoms are different, then that changes things. I'll show you how you can analyze this using the terminal atom, partial charge method.



Consider CH_3F . If you do Lewis and VSEPR, you will find that it is tetrahedral shape. At left, we see the partial charges for only the terminal atoms. The partial charges are not equal. This molecule is polar.

This example of CH_3F is fairly straightforward but others can get fairly complicated. Fortunately, for cases with different terminal atoms, there is a general fall-back position: by far, most cases are polar. That's not 100% true, but exceptions are fairly rare at this level.

Let me introduce a new term here: dipole or dipole moment. A dipole is another term for polarity as used here but it is also a quantitative measure. The term can be applied to a molecule or just to a bond. For example, we can say that a polar molecule has a dipole or we can say that a polar bond has a bond dipole. A dipole takes the symbol μ and its unit is called a debye ("*duh-BYE*"), which gets the symbol D. Values for μ have been measured for a vast number of compounds. Nonpolar compounds have no dipole so, for them, $\mu = 0$ D. Polar molecules will have some nonzero value; for example, the dipole moment is 1.85 D for H_2O and 1.86 D for CH_3F . Values for molecules can run up to 4 D or more. Dipole values are typically measured in the gas phase and these reflect a molecule's polarity by itself. Water's gas phase dipole is not real high but its liquid phase polarity is very high; that's measured differently.

Molecular polarity is an IMMENSELY important property and it has major impact in many areas in chemistry. It is important for you to be able to assess whether a molecule is polar or not. You need to work through this stuff. Try out other polarity problems. Here's a sampling of neutral molecules from the VSEPR Examples of this Chapter and Chapter 28. For each molecule, write in whether it is polar or nonpolar.

ClF_5 _____

ClF_3 _____

SiCl_4 _____

XeF_2 _____

SF_4 _____

AsCl_5 _____

I'll tell you that three are polar and three are nonpolar. You figure out which. If you really want to check, the answers are in Section 37.2.

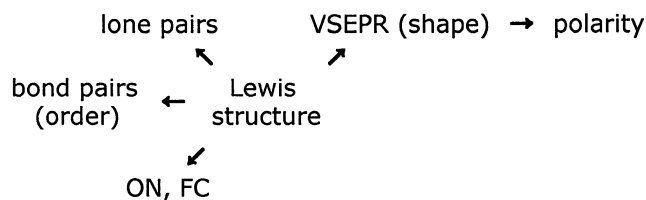
OK, I said I would mention two exceptions to assessing molecular polarity just as an illustration of how other factors can come into play. Here are the two: CO and NO. What's so exceptional about these?

Their molecular polarities are actually $C(\delta^-)\equiv O(\delta^+)$ and $N(\delta^-)=O(\delta^+)$, which is opposite to the bond polarities based on relative electronegativities. This is a rare occurrence, and these are the two most common cases. Although the molecular polarities are opposite to the bond polarities in these, it's not by much, and the dipole moments are very small at 0.11 D (CO) and 0.16 D (NO). So, yes, other factors can come into play to determine molecular polarity, but we stick with polarity based on electronegativities and shape for our purposes here.

29.6 Stage 3

Before closing out this Chapter, we can take our schematic to the next Stage. The Lewis structure directly provides information on all lone pairs and all bond pairs in the polyatomic unit. Also directly from the Lewis structure, we can determine oxidation numbers and formal charges. In addition, the Lewis structure is the lead into VSEPR for determining shape.

Once we know shape, we can determine a molecule's polarity. This schematic represents Stage 3. There's a lot here, but it's still not done.



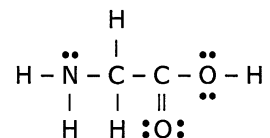
Problems

- What is the orientation of least repulsion and shape for each of the following classifications?
 - AX_4E_2
 - AX_4E
 - AX_5
 - AX_2E_3
 - AX_6
 - AX_3E_2
 - AX_5E

- What is the shape for each of the following?

- XeF_4
- ICl_2^-
- $SbCl_5$
- SiF_6^{2-}
- BrF_3

- Proteins are mostly composed of amino acids, the simplest of which is glycine, $C_2H_5O_2N$. The Lewis structure is at right. What is the shape for each of the central atoms?



- What are the ideal angles associated with each of the following?

- AX_2
- AX_3
- AX_4
- AX_5
- AX_6

- Which of the following will have bond angles less than the ideal angles? (Shapes for the first three were done in Chapter 28 Problems. Shapes for the other three are above.)

- $PF_3 \quad NF_4^+ \quad O_3 \quad XeF_4 \quad SiF_6^{2-} \quad BrF_3$

- Which of the following are polar? (Shapes for the first three were done in Chapter 28 Problems. Shapes for the other three are above.)

- $PF_3 \quad CO_2 \quad SeCl_2 \quad SbCl_5 \quad BrF_3 \quad XeF_4$

- Which of the following are polar?

- $Cl_2SO \quad XeO_2 \quad BBr_3 \quad BeF_2 \quad H_2CO \quad F_3ClO \text{ (O is equatorial.)}$