What makes a molecule polar or nonpolar?

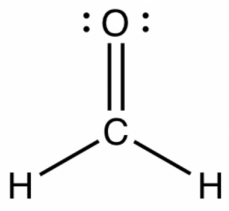
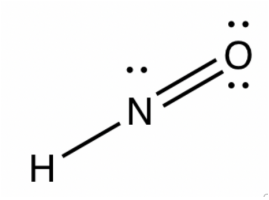
Developed by Ashley Ringer McDonald [1]

Information

Lewis Structures are essential tools chemists use to show how molecules that are inherently three-dimensional can be represented as two-dimensional. Since structure and function are closely linked VSEPR, or Valence Shell Electron Pair Repulsion, is a powerful tool for predicting the 3D structure using Lewis Structures. The guiding principle behind VSEPR is electron groups (regions of high electron density) around a central atom are coulombically driven to be as far apart from each other as possible. As a result, molecular geometries can be predicted by constructing a Lewis Structure and counting the number of electron groups around a given atom.

Counting electron groups around a central atom is relatively straightforward. For a given central atom,

$$\#\text{Electron Groups} = \#\text{Atoms Bound} + \#\text{Lone Pairs}. \tag{1}$$

H_2CO	HNO
	
C: 3 Atoms bound, 0 Lone Pairs	N: 2 Atoms bound, 1 Lone Pair
# Electron Groups = 3 + 0 = 3	# Electron Groups = 2 + 1 = 3

In each of the examples, there are 3 electron groups around the central atom. As a result, these molecules have the same electronic geometry or base geometry, trigonal planar (three electron groups spread out in a plane, separated by 120°). We will see that these molecules have different molecular geometries which show the shape based on the placement of atoms in space.

Part 1 Water

1. Sketch a Lewis structure for water. Count the number of electron groups and identify the electronic and molecular geometry.

2. Log on to WebMO with the credentials provided by your instructor.

[1]ORCID: 0000-0002-4381-1239, Department of Chemistry and Biochemistry, California Polytechnic State University

3. In the upper left hand corner, click New Job followed by Create New Job. It may take a few seconds to load.

4. Click the periodic table icon in the left column of icons. Choose oxygen. Click in the main building area on the screen to place an oxygen.

5. Go back to the periodic table and choose hydrogen. Click on the oxygen and drag to bond a hydrogen. Add another hydrogen to construct a water molecule. You don't have to worry about getting the bond lengths or bond angles correct at this time. The computer will calculate this for you.

6. Click the broom icon in the left column of icons. This will clean up your structure and create the correct bond angles and bond lengths.

7. Click the rotate arrow in the left column of icons. Rotate your molecule to study its three-dimensional shape. Does this match the shape you predicted from your Lewis Structure? Make a VSEPR sketch on your lab report form.

8. Click the right arrow at the bottom of the screen to advance. On the "Choose Computational Engine" page, select PSI4 and then click the right arrow to advance. In the next screen, give your job an appropriate name and fill in the following calculation details::

Job Name: "(yourinitials) H2O "
Calculation: Molecular Energy
Method: Hartree-Fock
Basis set: Routine: 6-311G(d)

9. Click the right arrow at the bottom of the screen to advance. The next screen will show you a list of all your jobs. The job you just created will say Running, Queued (meaning your job is waiting its turn to run), or Complete. If you job doesn't say Complete after a few seconds, refresh the page.

10. When your job says Complete, click the magnifying glass next to the word Complete. Your molecule will load in the window again. Scroll down to the Calculated Quantities section. On the sketch you drew in Step 7, label each atom with its partial charge.

11. Based on your partial charges, draw the bond dipole vectors on your sketch.

12. Study the 3D shape of the molecule on your screen and think about the bond dipole vectors. Do the bond dipole vectors cancel out or not? Predict if your molecule will a have a molecular dipole and the direction of the dipole moment vector.

13. Record the Dipole Moment for water. This is also found in the Calculated Quantities section. The units for dipole moment are Debye (D). Pay attention and make sure you record the exponent at the end of the number if there is one. Click on the magnifying glass next to Dipole Moment and it will show the direction of the dipole moment with a blue arrow on the molecule. Which way (towards positive or towards negative) does the dipole moment arrow point?

14. When you are finished recording all the information for water, click on Job Manager in the left column. This will return you to your list of all your jobs. You can now click New Job Create New Job in the upper left corner and build another molecule.

Part 2 Other molecules

15. For each molecule given below:

CH_4	NH_3	HCN
CO	H_2O	CH_3COOH (carboxylic acid)

a) Draw a Lewis Structure.

b) Identify the Electronic Geometry and Molecular Geometry.

c) Build the molecule in WebMO and make a VSEPR sketch.

d) On your VSEPR sketch, label the partial charges calculated from WebMO.

e) From the partial charges, draw the bond dipole vectors.

f) Thinking about the molecular shape and the bond dipoles, PREDICT if the molecule will have a molecular dipole and the direction of the dipole moment vector. Display the bond dipole vector in WebMO to check your prediction.

g) Record the dipole moment and draw the dipole moment vector on your sketch.

What makes a molecule polar or nonpolar?

Name _____ Date _____

Lab Partner _____

Part 1 Water

Lewis structure VSEPR sketch

1. Label the partial charges on your VSEPR sketch and draw the bond dipole vectors.

2. Record the dipole moment for water: _____

3. Which way (towards positive or towards negative) does the dipole vector point?

Part 2 Other molecules

4. CH_4

Lewis structure VSEPR sketch

Electronic Geometry: _____ Molecular Shape: _____

Dipole Moment: _____

5. CO_2

Lewis structure VSEPR sketch

Electronic Geometry: _____ Molecular Shape: _____

Dipole Moment: _____

6. HCN

Lewis structure VSEPR sketch

Electronic Geometry: _____ Molecular Shape: _____

Dipole Moment: _____

7. NH_3

Lewis structure VSEPR sketch

Electronic Geometry: _____ Molecular Shape: _____
Dipole Moment: _____

8. H_2O_2 For this molecule you can determine the geometry by considering either O the central atom.

Lewis structure VSEPR sketch

Electronic Geometry: _____ Molecular Shape: _____

Dipole Moment: _____

9. CH_3COOH For this molecule, identify the electronic geometry and molecular shape around each of the two carbons. Record your answers on the two sets of blanks below.

Lewis structure VSEPR sketch

Electronic Geometry: _____ Electronic Geometry: _____
Molecular Shape: _____ Molecular Shape: _____

Dipole Moment: _____

10. List any molecules that had a bond dipole, but did not have a molecular dipole. A molecule with no molecular dipole will have a very small (10^{-6} or less) dipole moment.

11. What do you notice about the shape of these molecules?