What makes a Molecule Polar?

Why are we doing this?

Contrary to the impression that Lewis structures may give, many molecules have three dimensional geometries. These molecular shapes are very important to understanding how molecules interact with each other, both chemically and physically. For example, the physical properties of a substance are dictated in part by whether or not the molecule is polar. For example, oil and water do not mix because water is polar whereas oil is nonpolar. Similarly, carbon dioxide is a solid at room temperature whereas water is a liquid at the same temperature because CO_2 is a nonpolar molecule while H_2O is polar. Using the shape of the molecule, we can explore the properties and arrangements of the bonds within those molecules. This will allow us to determine if a substance is polar or nonpolar.

Your Learning Outcomes

You will be able to:
1. Identify and use the trends of electronegativity.
2. Determine the polarity of a bond.
3. Determine the polarity of a molecule.
4. Describe and use the factors that influence the magnitude of the dipole moment for a molecule.

The Plan

1. Assign roles*.
    a. ***Manager*** – This person will keep the team on task and provide direction to the group. This person is responsible for uploading the group's work to Gradescope. Make sure you make a note of everyone in the group. You must add everyone's name when submitting your answers to Gradescope.
    b. ***Spokesperson*** – This person will represent the group be responsible for speaking for the group to the rest of the class.
    c. ***Recorder*** – This person will be responsible for recording the team's answers to the Critical Thinking Questions in an organized and coherent manner.
    d. ***Analyst*** – This person will be responsible for critical analysis of the team's work (i.e., the Devil's Advocate). This person should make sure everyone understands what is happening before the group moves forward.
2. Complete the Critical Thinking Questions as a group.
3. Submit your team's work via Gradescope. Groups may choose to work in a Word document or write out their answers on a separate sheet of paper. All work must be upload to Gradescope as a PDF file.

**Students may choose to complete this activity independently if they are unable to attend discussion due to illness or injury; in which case, the student must perform all roles and complete all aspect of the activity. To receive full credit, documentation as to the need for the absence from discussion must be included with the submission and your TA must be notified of the absence.*

Model 1: Electronegativities by Linus Pauling

Linus Pauling examined bonds between molecules such as H_2 and Cl_2 (called homonuclear diatomic molecules – molecules that are formed between two of the same atoms) and HF and HCl (called heteronuclear diatomic molecules – molecules that are formed between two different atoms). From this work, he proposed that the bonding electrons in heteronuclear molecules were not shared equally. Instead, one atom attracted the electrons in the bond more strongly than the other atom. Pauling called the ability of an atom (in a molecule) to attract electrons the **electronegativity**, χ, of the atom. In 1937, he devised a quantitative scale for electronegativity in which fluorine was assigned a value of about 4. This scale has since been refined based on more recent experimental evidence.

Table 1: Electronegativities for selected elements.

H 2.30								He 4.16
Li 0.91	Be 1.58		B 2.05	C 2.54	N 3.07	O 3.61	F 4.19	Ne 4.79
Na 0.87	Mg 1.29		Al 1.61	Si 1.92	P 2.25	S 2.59	Cl 2.87	Ar 3.24
K 0.73	Ca 1.03	Sc 1.2	Ga 1.76	Ge 1.99	As 2.21	Se 2.42	Br 2.69	Kr 2.97
Rb 0.71	Sr 0.96	Y 1.0	In 1.66	Sn 1.82	Sb 1.98	Te 2.16	I 2.36	Xe 2.58

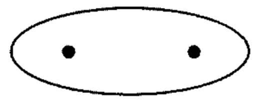
1. Describe the trend in electronegativities as you move from left to right across a period of the periodic table.
   Electronegativities tend to increase as one moves from left to right across a period of the periodic table.

2. Describe the trend in electronegativities as you move down a group of the periodic table.
   Electronegativities tend to decrease as one moves down a group of the periodic table.

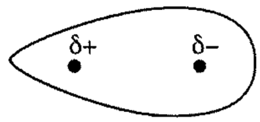
3. Compare the trends you identified above in Questions 1 and 2 to the corresponding trends in ionization energy.
   The trend in ionization energy is the same as the trend in electronegativity. This is reasonable because they both are a measure of how tightly an atom holds its electrons.

4. Explain why the partial charge on H in a molecule of HF is more positive than the partial charge on H in a molecule of HBr.
   F is more electronegative than Br. Therefore, the partial charge on F in HF should be more negative than the partial charge on Br in HBr. Thus, the partial charge on H in HF should be more positive.

Model 2: Polar and Nonpolar Bonds



A nonpolar bond is formed between identical atoms.



A polar bond is formed when there is an electronegativity difference between atoms.

5. Why do homonuclear molecules (H_2, N_2, O_2, and so on) have nonpolar bonds?
   The electronegativity of both atoms in a homonuclear diatomic molecule are the same. Therefore, they are pulling electrons evenly and creating a uniform distribution of charge (i.e., there are no more electrons on one side of the bond).

Model 3: The Dipole Moment

The polarity of the bond manifests itself in a measurable physical quantity called the dipole moment. A dipole moment, μ, is a vector quantity that has both magnitude and direction (bold letters are used for vector quantities).

$$\boldsymbol{\mu} = q \times \mathbf{d} \qquad \textbf{Equation (1)}$$

Where q is the magnitude of the two charges (one positive and one negative) and **d** is the distance (vector) between the two charges. The measured dipole for HCl is 1.03 D (D = debye, named after chemist Peter Debye; 1 D = 3.34 x 10^{-30} C m). The dipole moment can be represented by a vector; a plus sign is used to represent the center of the positive charge and the arrow tip represents the center of the negative charge. The measured dipole moment for HF is 1.82 D. Bond dipoles and dipole moments for HF, HCl, and H_2O are shown in Figures 1 and 2.

Figure 1. Bond dipoles and dipole moments for HF and HCl.

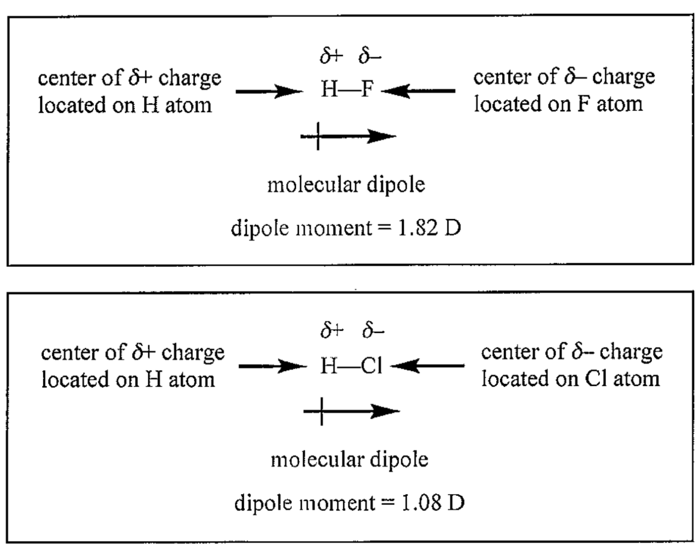
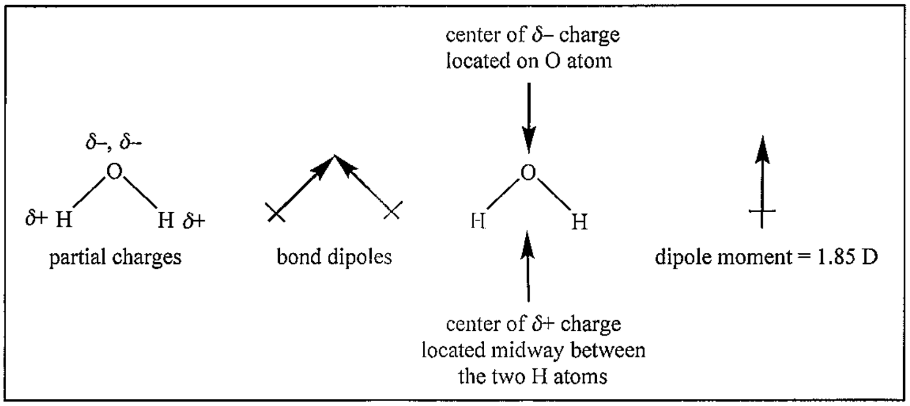


Figure 2. Bond dipoles and dipole moment for H_2O.



6. How was the center of the positive charge for the H_2O molecule, in Figure 2, determined?
   Both H atoms have the same partial charge (+). The center of positive charge is midway between the two H atoms.

Dipole moments for some other molecules are given in Table 2.

Table 2. Experimental dipole moments for selected molecules.

Molecule	Geometry	Polar Bonds	Dipole Moment (D)
H_2	Linear	No	0
HF	Linear	Yes	1.82
HCl	Linear	Yes	1.08
HBr	Linear	Yes	0.83
HI	Linear	Yes	0.45
CO_2	Linear	Yes	0
OCS	Linear	Yes	0.715
CH_4	Tetrahedral	Yes	0
CH_3Cl	Tetrahedral	Yes	1.892
CH_3Br	Tetrahedral	Yes	1.822
CH_3I	Tetrahedral	Yes	1.62
CF_4	Tetrahedral	Yes	0

7. The CO_2 molecule is linear (OCO) and has polar bonds.
   a. Where is the center of the positive charge?
      The center of positive charge is at the center of the C nucleus.

   b. Where is the center of the negative charge?
      The center of the negative charge is also at the center of the C nucleus.

   c. Why is the dipole moment for this molecule equal to zero?
      The distance between the center of positive charge and the center of negative charge is zero.

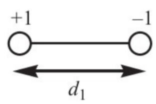
8. The CO_2 (OCO) and OCS molecules are both linear, and both have polar bonds. CO_2 does not have a dipole moment (that is, the dipole moment is zero). Why does OCS have a dipole moment?
   O is more electronegative than S. Therefore, the center of negative charge will not be at the nucleus of the C atom. There will be a distance between the center of positive charge and the center of negative charge.

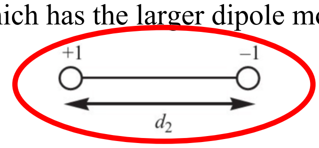
9. Consider the CF_4 molecule.
    a. Is each of the C-F bonds in CF_4 polar?
    Yes

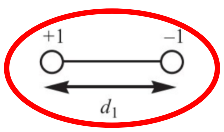
    b. Where is the center of the positive charge?
    The center of positive is located at the nucleus of the C atom.

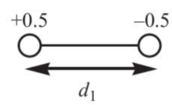
    c. Where is the center of the negative charge?
    The center of negative is located at the nucleus of the C atom.

    d. Why is the dipole moment zero for CF_4?
    The distance between the center of positive charge and the center of negative charge is zero.

10. Referring to Equation 1, which has the larger dipole moment in each of the following cases?
    a.
    

    b.
    

11. Consider HF and HCl:
    a. Which is the bigger atom, F or Cl?
    Cl is bigger than F (more shells)

    b. Which has the longer bond length, d, HF or HCl?
    HCl has the longer bond.

    c. Which has the greater partial charge – F in HF or Cl in HCl? (Hint: which is more electronegative – F or Cl?)
    F has the greater partial charge (is more electronegative).

    d. Why is the dipole moment of HF larger than the dipole moment of HCl? That is, which appears to be the more important factor in determining the dipole moment: The bond length or the partial charge?
    The partial charge appears to be a more important factor.

12. Based on the dipole moments for HF, HCl, HBr, and HI, in Table 2, which is more important un the determination of a dipole moment – the bond length (distance) or the electronegativity difference? Explain your reasoning.
The electronegativity difference—the d is larger for HI than for HF but HF has the largest dipole moment.