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Molecular Polarity

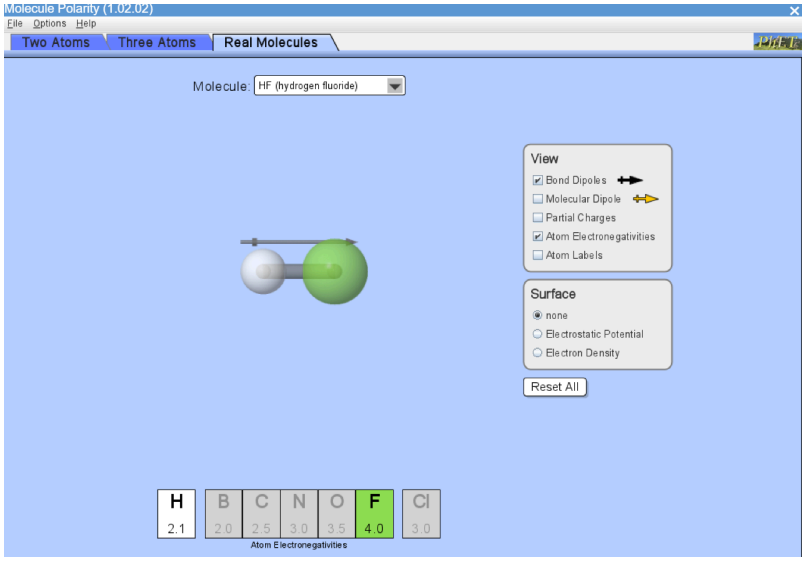
Introduction: Previously, we learned when a molecule will have covalent, ionic, or metallic character. We also learned about periodic trends, including electronegativity. Taking a closer look at covalent molecules, even though these molecules result from the sharing of electrons between atoms, sometimes these electrons will not be shared so evenly. What happens when one atom hogs more of the electrons in a bond? Today, we will conduct an investigation to find out!

Part 1: Demo

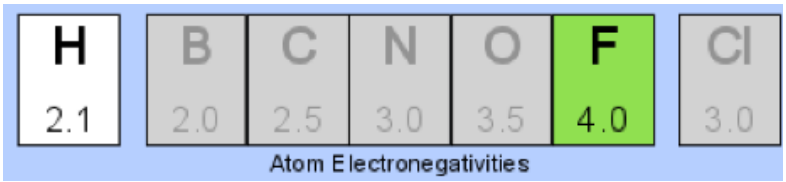
1. Write your observations below.
   There seems to be like static electricity. Also the water is bending towards the pipe
2. Why do you think the water is bending towards the PVC pipe?
   Maybe because of the static electricity.

Part 2:

1. Google "molecule polarity phet" and click on the first option. Alternatively, follow this link.
2. Start the sim and select the "Real Molecules" portion, which is currently only available for Java. Be patient as it will take a moment for the sim to load.
3. Choose the "Real Molecules'' tab at the top of the sim. You should start with the molecule HF (hydrogen fluoride). On the View window, check only "Bond Dipoles" and "Atom Electronegativities." Currently, you should have the "None" radio button selected on the Surface window.

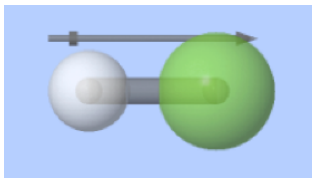


- Note the "Atom Electronegativities" key presented to you at the bottom of the simulation window:



Questions:

1. Take a look at the molecule in the simulation:



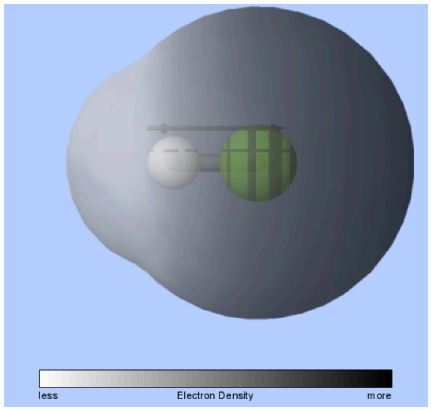
   a. Which atom is hydrogen, and which one is fluorine?

Green - Flourine, Gray, Hydrogen

   b. Which atom has a higher electronegativity?

Flourine

2. Notice the gray arrow hovering above the molecule. As discussed in class, we use that arrow to signify shifts in electron density. Towards the head of the arrow is greater electron density and towards the tail is lesser electron density. In other words, the bond is slightly more negative towards the head and slightly more positive towards the tail. You can also visualize the electron density in this molecule by checking the "Electron Density" radiobutton on the Surface window. The following visual should appear:



   a. For HF (hydrogen fluoride), towards which atom does the arrow point?

Fluorine

   b. Which side of the molecule is more negative? Which side is more positive?

Fluorine more negative, Hydrogen more positive

   c. Around which atom is there more electron density in HF?

Fluorine

3. Repeat this process with other molecules. Record your data in the table below:

Molecule	Atom 1	Atom 1 electronegativity	Atom 2	Atom 2 electronegativity	Near which atom is there more electron density?
Hydrogen Fluoride (HF)	H	2.2	F	4.0	F
Water (H_2O)	H	2.2	O	3.44	O
Carbon dioxide (CO_2)	C	2.5	O	3.44	O
Ammonia (NH_3)	H	2.2	N	3.0	N
Borane (BH_3)	B	2.0	H	2.2	H

a. Is there a pattern between the electronegativity values and the atom with greater electron density?

The higher electronegativity atoms have more electron density

4. Let's test the pattern you came up with in 3(a) for the following molecules:
   a. Boron (B) has an electronegativity value of 2.0, and fluorine (F) has an electronegativity value of 4.0. Imagine there is a molecule containing both of these elements, BF_3 (boron trifluoride). According to the pattern you came up with in the previous activity, near which atom should there be more electron density? **Do *not* check this on the simulation yet!**

Fluorine

   b. According to the pattern you came up with, make similar predictions for two other molecules, methane (CH_4) and tetrafluoromethane (CF_4) and fill in the table below.

Molecule	Atom 1	Atom 1 electronegativity	Atom 2	Atom 2 electronegativity	Near which atom ***should*** there be more electron density?
Boron trifluoride (BF_3)	B	2.0	F	4.0	Fluorine
Methane (CH_4)	C	2.55	H	2.2	Carbon
Tetrafluoromethane (CF_4)	F	4.0	C	2.55	Fluorine

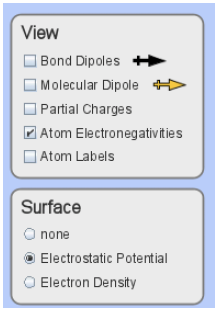
c. Let's check if your predictions that you made in 4 (b) match the outcomes in the simulation:

Molecule	Near which atom ***is*** there more electron density?	Did the outcome match your prediction?
Boron trifluoride (BF_3)	Fluorine	✓
Methane (CH_4)	Carbon	✓
Tetrafluoromethane (CF_4)	Fluorine	✓

d. According to the results of this testing experiment, what judgment can you make about the pattern you came up with? Was it supported or disproved?

The pattern was upheld correctly

In the previous activities, you found a pattern between the electron density in a molecule and the electronegativity differences of the atoms in that molecule. The idea of having different electron densities distributed between atoms in a molecule has a name: **polarity**. When electrons are not distributed symmetrically within a bond, that bond is polar (i.e. HF). What if we were to extend this idea to molecules? *When electrons are not distributed symmetrically within a molecule, that molecule is called "**polar**." When electrons are distributed symmetrically within a molecule, that molecule is called "**nonpolar**."* Let's explore this idea via the simulation!

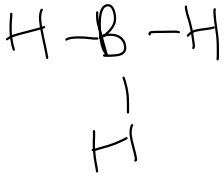


5. On the PhET simulation, make sure the following options are checked: On the View window, only "Atom Electronegativities" should be checked. This is so you can continue to identify which atom is which in the molecule. On the Surface window, only "Electrostatic Potential" should be checked.

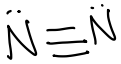
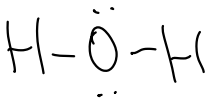
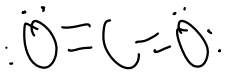
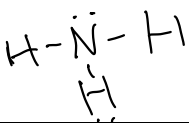
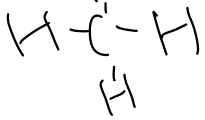
6. The simulation already tells us if a molecule is polar or nonpolar. If the molecule is polar, it will have distinct red or blue regions. However, if the molecule is nonpolar, it will have more muted colors.
   a. Compare HF to BH_3. Which one is polar, and which one is nonpolar?

HF is polar while BH_3 is nonpolar

   b. Clearly, H and F have different electronegativity values, but so do H and B. What might be able to explain why one is polar whereas the other is not? Start by drawing a Lewis structure for each.

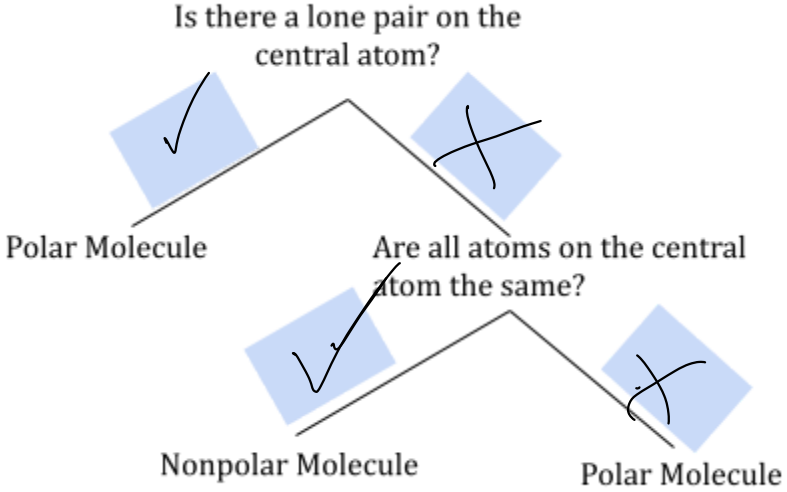


7. Let's continue to take a look at other molecules.
    a. Fill in the following table with your observations from the simulation.

Molecule	**Lewis Structure**	**Which element is more negative?**	**Are the <u>bonds</u> in this molecule polar or nonpolar?**	**Is the <u>molecule</u> polar or nonpolar?**
Nitrogen (N_2)		They're the same??	They are polar nor	The molecule is nonpolar
Water (H_2O)		O	polar	nonpolar
Carbon dioxide (CO_2)		O	polar	nonpolar
Ammonia (NH_3)		N	polar →	→
Methane (CH_4)		Same again?	nonpolar →	→

    b. Based on your observations and your drawn Lewis structures, is there a pattern between the Lewis structure for a molecule and whether that molecule is polar or nonpolar? Let's come up with a set of rules to determine when a molecule is polar or nonpolar…

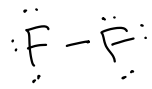
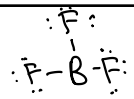
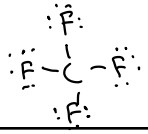
        i. In the shaded text boxes on the following flowchart, write YES or NO, keeping in mind which box leads to"polar molecule" or "nonpolar molecule":



8. In the previous activity, you came up with a set of possible rules to determine when a molecule is polar or nonpolar.

    a. Using these rules you developed and drew Lewis structures to help you predict whether the following molecules will be polar or nonpolar.

    b. **<u>After</u>** you make your predictions, check the outcomes on the simulation.

Molecule	**Lewis Structure**	**Prediction: Should the <u>molecule</u> be polar or nonpolar?**	**Outcome: According to the simulation, is the <u>molecule</u> polar or nonpolar?**
Fluorine (F_2)		Nonpolar →	
Boron trifluoride (BF_3)		Nonpolar →	
Tetrafluoromethane (CF_4)		Nonpolar →	

    c. Did your predictions match your outcomes? What judgment can you make about the set of rules you developed for deciding when a molecule is polar or nonpolar?

<u>Reflection: Demo Again</u>

1. Why is the water bending towards the PVC pipe?

Because of the imbalance in between the charges. And the fact that the water molecules are polar.