ROSEDALE ACADEMY

1-5: Molecule Polarity Lab

A study of electronegativity, bond polarity, and molecular polarity

Instructions: Click on the link provided on the assignment page or go to: http://phet.colorado.edu/en/simulation/molecule-polarity and click run.

Introduction:

In this atomic-level simulation, you will investigate how atoms' ***electronegativity*** value affects the bonds they produce. When two atoms bond, a pair of electrons is shared between atoms. Electronegativity is a measure of a single atom's ability to hoard electrons shared in that bond.

Part 1 - Procedure:

- Begin with the 2 atoms tab on the top
- Turn on (check) all view options and electron density.
- Take your time and investigate how the compound's bond behaves when the atom's electronegativity and orientation are changed. Do not rush through this step.

1. Describe the bond formed between two atoms with **similar, low** electronegativities.

   Answer: **Covalent**

2. Describe the bond formed between two atoms with **similar, high** electronegativities.

   Answer: **Covalent**

3. Describe the bond formed between two atoms with **very different** electronegativities.

   Answer: **Ionic**

4. δ- represents: **A negative dipole**

5. δ+ represents: **A positive dipole**

6. What happens when the electric field is applied to a very polar molecule?

   The molecule orients itself in the magnetic field with the negative dipole at the positive side of the electric field and the positive dipole at the negative side of the electric field.

7. Why do you think this is?

   The negative dipole is attracted to the positive side of the electric field and the positive dipole is attracted to the negative side of the electric field. Alternatively, the negative dipole is repelled by the negative side of the electric field, while the positive dipole is repelled by the positive side of the electric field.

8. What is **electron density**?

Electron density shows where there is a higher concentration of electrons. Across a bond, when one atom is more electronegative than another it tends to pull the electrons shared between them towards it. Therefore the more electronegative atom will have a higher electron density while the less electronegative atom will have a lower electron density.

9. How does the density around a partial positive compare to the density of a partial negative?

There is a higher electron density around a partial negative compared to a partial positive.

10. What would bring about a higher electron density around an atom?

A higher electronegativity value would cause an increase in electron density.

11. A bond is characterized as ionic or covalent by comparing the differences between two atoms' electronegativities. Describe an ionic bond in terms of the atoms' electronegativity values.

In an ionic bond, one of the atoms must have a higher electronegativity value than the other atom across the bond. The difference in electronegativity values must be 1.7 or greater.

12. Describe a covalent bond in terms of the atoms' electronegativity values.

In a covalent bond the difference in electronegativity values between atoms on either side of a bond must be relatively low. Specifically the difference in electronegativity values must be less than 1.7 to be considered covalent.

13. Additionally, we further separate covalent bonds into ***polar*** *covalent* and ***nonpolar*** *covalent*. What would have to be the case for a bond to be *nonpolar covalent*?

In a non-polar covalent bond the electrons are shared almost entirely equally between atoms on either side of the bond. Specifically, to be considered non-polar covalent, the difference in electronegativity values must be less than 0.5.

Part 2 - Procedure:

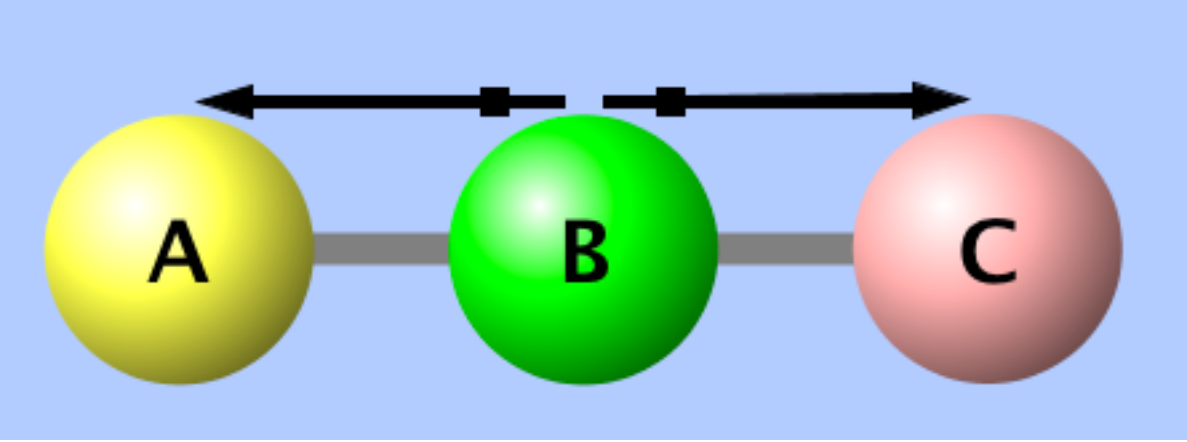
- Click on the "Three Atoms" tab at the top of the simulator
- Check all the view options

In this simulation realize that in addition to changing the electonegativities, you may also move individual atoms by dragging them with the mouse. Here, in addition to bond polarity (represented by the ***bond dipole***), the ***entire molecule may be polar*** (represented by the ***molecular dipole***). It is this molecular dipole that determines the polarity of the molecule and how it interacts with other molecules and its environment.

❖ Take some time and adjust each of the atom's locations and electronegativity values several times. Observe how the bond dipoles (between A-B and B-C) add to produce a molecular dipole.

1. How might a molecule with two strong bond dipoles have no molecular dipole at all?

If a molecule is symmetrical, for example, a 3-atom molecule that is linear, it is possible for there to be 2 strong bond dipoles but no net overall molecular dipole. In the image below, A and C both have high electronegativity values relative to B. Therefore the A-B bond and A-C bond have strong bond dipoles. But because the molecule is symmetrical, these two bond dipoles essentially cancel each other out, therefore there is no net molecular dipole for this molecule.



2. How might a molecule have a very strong molecular dipole?

A molecule can have a very strong molecular dipole if there is one or more strong bond dipoles that do not cancel each other out due to symmetry. In the image below, A and C once again have high electronegativity values, and therefore the A-B bond and A-C bond have strong dipoles. But because of the shape of the molecule, the 2 dipoles do not cancel each other out, but instead cause the molecule itself to have a very strong molecular dipole.