

# Molecule Polarity PhET Lab

Name: Key 2023

Related to Objective 5: A study of electronegativity, bond polarity, and molecular polarity.

## Introduction:

tendency of an atom to attract  $e^-$

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. In this lab you will work diligently, at your own pace, to answer a number of questions. To begin, from what you've already learned about the protons and electrons in an atom, what would cause an atom to have a **high** electronegativity value?

When an atom has more valence  $e^-$ , EN will be higher

Why might an atom have a **low** electronegativity value?

When an atom has fewer valence  $e^-$ , EN will be lower

## Procedure: Two Atoms

- ❖ Turn on (check) all view options.
- ❖ Take your time and investigate how the binary compound's bond behaves when the atom's electronegativity and orientation are changed. Do not rush through this step.

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

more covalent

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

more covalent

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

more ionic

Describe (in your own words) what is meant by **partial charges**,  $\delta^-$  and  $\delta^+$ . not completely + or -

$\delta^-$  represents:  $e^-$  are more densely concentrated to this side

$\delta^+$  represents:  $e^-$  are less densely concentrated to this side

What happens when the electric field is applied to a very polar molecule? molecule aligns to magnetic field

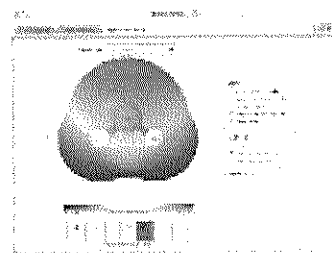
Why do you think this is? partial - is attracted to the + and vice versa

What is **electron density**? how close the  $e^-$  are likely to be to each other

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

density around  $\delta^+$  is less than density around  $\delta^-$

What would bring about a higher electron density around an atom? unequal EN values



Molecule Polarity

**View**

Bond Dipole  $\leftrightarrow$

Partial Charges

Bond Character

**Surface**

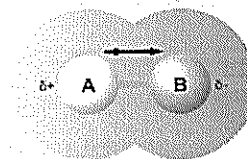
none

Electrostatic Potential

Electron Density

**Electric Field**

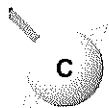
on  off



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. Large EN diff 1.7 or ↑

Describe a covalent bond in terms of the atoms' electronegativity values. Smaller EN diff 0-1.7

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**? Very similar or identical EN values



### Three Atoms

In this simulation, realize that in addition to changing the electronegativities, 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. For instance, molecules with high molecular dipoles tend to have high **intermolecular forces**. (Why?)

0-0.4

### View

- Bond Dipoles  $\leftrightarrow$
- Molecular Dipole  $\leftrightarrow$
- Partial Charges

### Electric Field

- on  off

BTW: The molecular dipole is found using **vector addition**, adding the bond dipoles together; think a *tug-of-war*.

- ❖ 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.

How might a molecule with two strong bond dipoles have no molecular dipole at all? bonds may be polar but molecule is symmetrical

How might a molecule have a very strong molecular dipole. large EN diff, asymmetrical

### Real Molecules

"Like dissolves like" is a way to remember that molecules with **similar molecular dipoles** will tend to interact favorably and mix. For instance, water (H<sub>2</sub>O) is a polar molecule. It will mix well (dissolve) polar molecules, such as ammonia (NH<sub>3</sub>), a mixture often used in household cleaners. Both molecules possess strong molecular dipoles. A molecule such as methane (CH<sub>4</sub>) would not dissolve well into water. Why? weak molecular dipole (nonpolar molecule)

**Before using the simulation**, complete the table below (with a  $\checkmark$ ) to predict which of the following should dissolve into water. Create a Lewis-dot diagram ( $:\ddot{O}=C=\ddot{O}:$ ) for each to guide your thinking. (use a separate page)

**Prediction (before using the simulation)**

H <sub>2</sub>	N <sub>2</sub>	O <sub>2</sub>	F <sub>2</sub>	HF	H <sub>2</sub> O	CO <sub>2</sub>	HCN	O <sub>3</sub>	NH <sub>3</sub>	BH <sub>3</sub>	BF <sub>3</sub>	CH <sub>2</sub> O	CH <sub>4</sub>	CH <sub>3</sub> F	CH <sub>2</sub> F <sub>2</sub>	CH <sub>3</sub> F	CF <sub>4</sub>	CHCl <sub>3</sub>
				✓	✓		✓		✓			✓		✓	✓	✓		✓

<<Optional>> Next, use the simulation to determine with of the species should dissolve in water.

H <sub>2</sub>	N <sub>2</sub>	O <sub>2</sub>	F <sub>2</sub>	HF	H <sub>2</sub> O	CO <sub>2</sub>	HCN	O <sub>3</sub>	NH <sub>3</sub>	BH <sub>3</sub>	BF <sub>3</sub>	CH <sub>2</sub> O	CH <sub>4</sub>	CH <sub>3</sub> F	CH <sub>2</sub> F <sub>2</sub>	CH <sub>3</sub> F	CF <sub>4</sub>	CHCl <sub>3</sub>
					✓													

Finally, what type of solvent would be required to dissolve **nonpolar** compounds? \_\_\_\_\_