Molecule Shapes and Inter Molecular Forces

**Introduction**

Atoms bond to satisfy their need for more electrons. If both atoms have high electro-negativities (are nonmetals), atoms will share electrons to satisfy the Octet Rule – every atom wants 8 electrons to fill the s and p orbitals in the outer energy level. But, as you will see, if the electro-negativities are high enough and both atoms unwilling to give up electrons, sometimes atoms can deviate from and not follow) the Octet Rule.

Prelab:

Define following terms in your lab note book:

1. VSEPR
2. Electronegativity
3. Octet Rule
4. Exception to octet rule
5. Electron domain
6. Electron geometry
7. Molecular geometry
8. Bond dipole
9. Molecule polarity

**Molecule Shapes**

Log on to <https://phet.colorado.edu/en/simulation/molecule-shapes> either by Googling “phet simulations molecule shape.” Click on “***Run Now***.” If a screen pops up asking to update Java, click on “***Later***.”

Part 1: Electron domains

Explore the *Model* screen of the simulation and check what happens to existing atoms/lone pairs

* 1. when you add an atom or lone pair
	2. when you remove an atom or lone pair,
	3. does adding an atom have same effect as adding a lone pair?

Part 2: 3D Drawings

* Line: In the plane of the paper: **\_\_\_\_\_**
* Wedge: Coming forward, in front of the plane of the paper: 
* Dash: Going backward, behind the plane of the paper: 
1. ****Draw the molecule of CHFClBr on left in your notebook and label the position of each atom as
* In the plane of the paper \_\_\_\_\_\_ \_\_\_\_\_\_ \_\_\_\_\_\_
* In front of the plane of the paper \_\_\_\_\_\_
* Behind the plane of the paper \_\_\_\_\_\_

1. Using the *Model* screen, add bonding domains (●) to the central atom (○). Using lines, wedges and dashes, draw each molecule’s shape. Draw table in your lab notebook. Note: Bonding domains include any kind of bond and lone pairs.

|  |  |  |  |
| --- | --- | --- | --- |
| Bonding Domains Around Central Atom | Drawing of Shape | Electron Geometry | Bond Angeles |
| 2 | ●-○-● | Linear | 180° |
| 3 | ○ |  |  |
| 4 | ○ |  |  |
| 5 | ○ |  |  |
| 6 | ○ |  |  |

1. In the *Model* screen, build a molecule with 5 atoms attached to the central atom. Look at the molecule geometry and electron geometry. **Predict** what will happen to the molecule geometry as you replace atoms with lone pairs. Was your prediction correct? Explain in terms of valence shell electron pair repulsion theory.

**Part 3 – Generic Molecules**

Creating 10 generic molecules below. On your screen in the lower left corner, click on “***molecule geometry***.” Add atoms and electron pairs as needed to produce the generic formula. Once the molecule is assembled, click and drag the screen to spin the atom around. Click on the “***Show bond angles***.” Use the following key:

* ***A*** – **central purple atom**
* ***B*** – single bonded white atom
* ***C*** – double bonded white atom
* ***D*** – triple bonded white atom
* ***E*** – Electron pairs not bonded

List of generic molecules: AC2, ABE3, AB3E, AB, ACE2, AB2E2, AB2C, AB3, AB4, ADE

For each generic molecule:

1. Draw the molecule you create to the best of your ability
2. Write the Molecule Geometry name
3. Label the bond angle
4. Look at the central atom, is its octet satisfied? Label to show that.

**Part 4 – Real Molecules**

Click on the “***Real Molecules***” tab at the top of the page. Using the pull down menu, select the molecules below and fill in the chart. Match the molecule to the generic structure above. Fill in the generic bond angles.

|  |  |  |  |
| --- | --- | --- | --- |
| Molecule | Generic Formula | Generic bond angles (from part 3 ) | True Bond Angles |
| H2O |  |  |  |
| CO2 |  |  |  |
| CH4 |  |  |  |
| NH3 |  |  |  |
| BF3 |  |  |  |

**Part 5 – Octet Rule Breakers**

While still in the “**Real Molecules**” tab, select the following molecules. Draw each molecule, name the geometry and write how many electrons are on the central atom.

SO2, XeF2, ClF3, SF4, XeF4, BrF5, PCl5, SF6

Exceptions to the octet rule fall into one of three categories: (1) incomplete octet, (2) odd-electron molecules, and (3) an expanded octet.

Incomplete Octet: In some compounds, the number of electrons surrounding the central atom in a stable molecule is fewer than eight.  Beryllium is an alkaline earth metal and so may be expected to form ionic bonds.  However, its very small size and somewhat higher ionization energy compared to other metals actually lead to beryllium forming primarily molecular compounds.  Since beryllium only has two valence electrons, it does not typically attain an octet through sharing of electrons.

Odd-Electron Molecules: There are a number of molecules whose total number of valence electrons is an odd number.  It is not possible for all of the atoms in such a molecule to satisfy the octet rule.  An example is nitrogen dioxide (NO2).  Each oxygen atom contributes six valence electrons and the nitrogen atom contributes five for a total of seventeen.

Expanded Octets: Atoms of the second period cannot have more than eight valence electrons around the central atom.  However, atoms of the third period and beyond are capable of exceeding the octet rule by having more than eight electrons around the central atom.  Starting with the third period, the d sublevel becomes available, so it is possible to use these orbitals in bonding, resulting in an expanded octet.

**MOLECULE POLARITY**

<https://phet.colorado.edu/en/simlation/legacy/molecule-polarity>

**Part 6: Two atoms screen**

1. Explain **all the ways** you can change the polarity of the two-atom molecule.
2. Draw this table in your notebook

|  |  |  |
| --- | --- | --- |
| Representation | Response to change in electronegativity | Effect on molecule polarity |
| Bond Dipole |  |  |
| Partial Charges |  |  |
| Electrostatic Potential |  |  |

**Part 7: Three atoms screen**

1. Explain any **new** ways to change the molecule polarity of the three-atom molecule.
2. How does the **ABC-bond angle** effect molecule polarity? Tip: Try changing the bond angle in the simulation.
3. Explain the relationship between the **bond dipoles** and the **molecule dipole**.
4. Can a non-polar molecule contain polar bonds? Use an **example** to explain your answer.

**Part 8: Real Molecules**

**Check** the polarity of eight real molecules in the simulation. Four have been picked for you and pick one more from two atoms, 3 atoms, 4 atoms and 5 atoms group.

For each molecule:

1. Draw molecule including bond angles, bond dipoles and Molecule dipoles. Color code your drawing by using same color for the atoms as in simulation, green arrows for bond dipoles and Bold red for molecule polarity
	1. HF
	2. H2O
	3. BF3
	4. CHCl3

**Post Lab Questions**

1. What does **VSEPR** stand for? Explain its meaning in your own words. (not same as prelab)
2. The program did not give a bond ***angle*** to a molecule consisting of only two atoms. Why? Think geometry class.
3. Comparing real molecules to generic molecules in Part 4, some of the angles stayed consistent while others did not. Compare and contrast the two groups of molecules (*those with matching angle measurements* to *those with different measurements*). What is causing the angles to skew? Explain why this might be.
4. What angle is needed to spread 4 bonds as far apart as possible? Hint: look at a molecule with four separate bonds.