

Reading assignment: Chang, Chemistry 10th edition, pages 380-385, 410-419.

Goals

We will study molecular structure through molecular models as well as become familiar with VSEPR geometries and the effect of molecular geometry on polarity.

Building Molecular Models

Students work in pairs using a molecular model kit.

Molecular models are used to build representations of covalent molecules. Balls are used to represent atoms and sticks are used to represent chemical bonds. We will use a kit with five colors used to represent nonmetal atoms. Use the following color code when constructing models:

White– hydrogen

Red– oxygen and sulfur

Black– carbon, boron, and silicon

Green– fluorine, chlorine, bromine, and iodine

Blue– nitrogen and phosphorus

Yellow–sulfur (hexavalent)

Purple– phosphorus (pentavalent)

There are also two components in the kit used to represent chemical bonds:

- The short gray pieces are used to represent single bonds between atoms not including hydrogen.
- The long flexible gray pieces are used to represent double and triple bonds between atoms.

VSEPR

In determining the geometric structures of small molecules we will use the valence-shell electron-pair repulsion (VSEPR) model. The VSEPR model is based on the Lewis model of covalent bonding. The strategy for determining geometric structures is to first draw the Lewis structures for all of the atoms in the molecule. Covalent bonds are then formed between the central atom and the surrounding atoms. The geometric structure of the molecule is then determined by minimizing electron-pair repulsion in the Lewis structure. The number of valence electrons (VE) for each atom is found from the periodic table.

Number of valence electrons							
1	2	3	4	5	6	7	8
H	He						
Li	Be	B	C	N	O	F	Ne
Na	Mg	Al	Si	P	S	Cl	Ar
K	Ca	Ga	Ge	As	Se	Br	Kr

Example: methane CH₄ Lewis structures of individual atoms $\cdot\overset{\ominus}{\underset{\oplus}{\text{C}}}\cdot$ $\cdot\text{H}$

Lewis structure of molecule:

```

      H
      |
H — C — H
      |
      H
    
```

In methane there are four electron domains (ED) around the central atom, each a bonding electron pair to a hydrogen atom. The domains will arrange themselves to minimize electron-pair repulsions. The relationship between the number of electron domains and geometric arrangement is shown below. Note that double and triple bonds each count as one electron domain around the central atom.

ED

Angle

2	180°
3	120°
4	109.5°
5	90° and 120°
6	90°

Four electron domains will, therefore, result in angles of 109.5°. The geometric structure of the molecule is determined by considering the arrangement of atoms and can be determined from the number of electron domains (ED) and number of surrounding atoms around the central atom. Common structures include:

ED	Number of surrounding atoms					
	1	2	3	4	5	6
2	linear	linear	-----	-----	-----	-----
3	linear	bent	trigonal planar	-----	-----	-----
4	linear	bent	trigonal pyramidal	tetrahedral	-----	-----
5	-----	linear	T-shaped	distorted tetrahedral	trigonal bipyramidal	-----
6	-----	-----	-----	square planar	square pyramidal	octahedral

Methane will have a tetrahedral arrangement because it consists of four electron domains and four surrounding atoms. Another example is ammonia (NH₃), a molecule with four electron domains around the central atoms and three surrounding atoms. From the table above ammonia will have a trigonal pyramidal geometry.

Procedure

Part 1: Building Models

Select at least ten molecules and ions from the list below and construct molecular models for each of them. Before building the model construct a Lewis structure for the molecule and then predict the geometric structure of the molecule based on VSEPR theory.

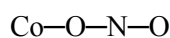
H ₂ O	C ₂ H ₄	CH ₄	C ₂ H ₂	CO ₂	HNO ₃ *	SF ₂
H ₂ CO ₃ *	NH ₃	N ₂	PH ₃	HCN	CH ₂ Cl ₂	CH ₄ O
BF ₄ ⁻	PCl ₅	NH ₄ ⁺	C ₆ H ₆ **	C ₃ H ₈	CH ₂ O	SF ₆

* Hydrogen atoms are bonded to oxygen atoms.

** The carbon atoms form a 6-membered ring with three double bonds between carbon atoms in the ring. If the element symbol is in bold then it's the central atom.

Part 2: Isomers

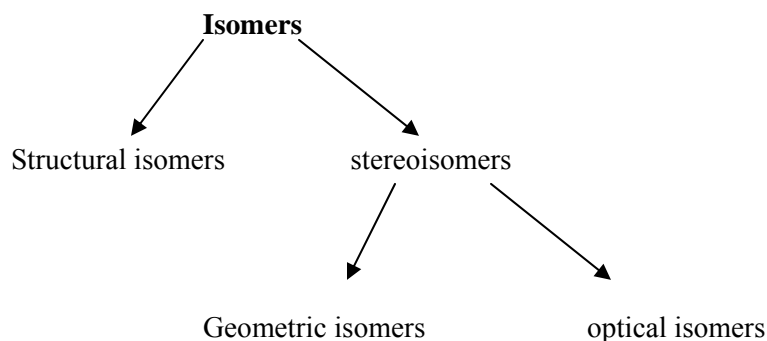
Isomers are compounds that have the same chemical formula but have different properties, based on the arrangement of atoms or chemical bonds. Isomers are classified as either structural isomers or stereoisomers. Structural isomers differ as a result of differences in how atoms are bonded. For example, consider the bonding of cobalt to nitrite (NO₂⁻):





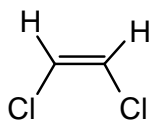
In the first structure cobalt is bonded to nitrogen. In the second structure cobalt is bonded to oxygen. This difference will lead to physical differences between the two compounds.

Stereoisomers differ as a result of differences in the spatial arrangement of atoms. There are two categories of geometric isomers we will consider in detail: Geometric isomerism and optical isomerism.

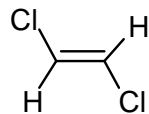


Geometric Isomerism

Build models of the two molecules (dichloroethene) shown below:



cis-dichloroethene

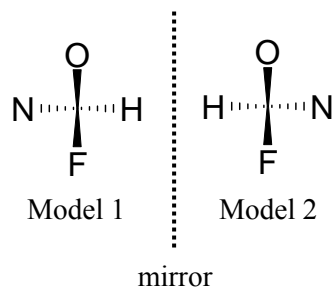




trans-dichloroethene

These two molecules are very similar to one another. They differ only in that in the first molecule the two chlorine atoms are on the same side (cis) of the carbon-carbon double bond. In the second molecule the two chlorine atoms are on opposite sides (trans) of the carbon-carbon double bond. Although these two molecules possess the same molecular formula and molar mass they differ in several physical properties. The trans form of 1,2-dichloroethene has a melting point of -49.4°C and a boiling point of 47.7°C . The cis form has a melting point of -81.5°C and a boiling point of 60.2°C . Cis-1,2-dichloroethene is more soluble in water at 7.7 g/L compared to 6.3 g/L for the trans isomer.

Optical Isomerism

Build two models in which carbon is the central atom and with four different substituents. For example, oxygen, nitrogen, hydrogen, and fluorine. When you build the two models place them next to each other. The hydrogen atoms should be facing each other and the nitrogen atoms should be pointing away from each other as if the second model were a mirror image of the first. Three-dimensional representations of these models are shown below.



Where  means that the bond projects out of the paper and  means that the bond projects into the paper.

Compare the two molecules. Are they identical? There are a couple of ways we can compare the two structures.

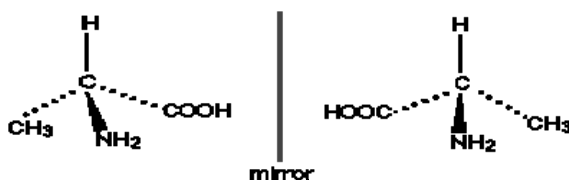
Test 1: One way to answer this question is to measure the distances between the atoms. For example, is the distance between the nitrogen and fluorine atoms the same in each model?

Test 2: Compare the angle between the carbon atom and any two surrounding atoms for each model. For example, F-C-O. Are the angles in each model identical or different?

For the models you just built the answer should be yes. Both structures should also have nearly identical physical and chemical properties because their structures are so similar. But the two structures are different in one significant way.

Test 3: Try to rotate one of the models so that all atoms line up together: N to N, O to O, H to H, and F to F. If the two models can be lined up then models 1 and 2 are completely identical and represent the same molecule. If the two models cannot be lined up, then there is a difference.

Structures 1 and 2 are mirror images of each other, like a right hand compared to a left hand. They are two different molecules. One of the two molecules will rotate the plane of polarized light to the right while the other will rotate the plane of polarized light to the left and are called optical isomers. One of the isomers is called dextro and the other isomer is called levo. Levo and dextro are often abbreviated "l" and "d." This effect on polarized light is the only physical property in which the two structures differ. Many molecules important in biology exhibit this physical property. An example is the amino acid alanine. In alanine the central carbon atom is surrounded by four constituents: -CH₃, -NH₂, -COOH, and -H

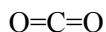


l-alanine and d-alanine

Part 3: Qualitative Study of Polar and Nonpolar Molecules

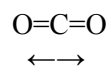
Chemical bonds are polar based on electronegativity differences between atoms in the bond. Electronegativity values are shown in the table below for selected elements. The F-H bond is very polar because fluorine has an electronegativity value of 4.0 and hydrogen has a significantly smaller value of 2.1.

Determining the polarity of molecules is more complicated. Knowledge of the bond polarities and of the arrangement of atoms in the molecule are required. For example, carbon dioxide is a nonpolar molecule even though it possesses two strongly polar bonds:



H						
2.1						
Li	Be	B	C	N	O	F
1.0	1.5	2.0	2.5	3.0	3.5	4.0
Na	Mg	Al	Si	P	S	Cl
0.9	1.2	1.5	1.8	2.1	2.5	3.0
K	Ca	Ga	Ge	As	Se	Br
0.8	1.0	1.6	1.8	2.0	2.4	2.8
Rb	Sr	In	Sn	Sb	Te	I
0.8	1.0	1.7	1.8	1.9	2.1	2.5

Arrows can be used to represent the polarity of each bond. In this notation the head of the arrow points in the direction of the more electronegative atom in the bond. For CO₂:



So the lack of polarity in CO₂ is a result of the geometric arrangement of its atoms. The polarity of each carbon-oxygen bond is effectively cancelled by the other due to the directional nature of polar bonds.

$\leftarrow\rightarrow$ (cancellation results in no net polarity)

Procedure

1. Draw the Lewis structures for the molecules in the table on the data sheet.
2. Then build a model of each molecule and predict whether the molecule will be very polar, somewhat polar, or nonpolar based on the bond polarities and the geometric arrangement of atoms.

Steps 3-8 may be performed as a demonstration.

3. In the hood there is a pasteur pipette attached by a clamp to a ringstand. There is also a beaker under the pipette to catch liquids that flow through the pipette.
4. Vigorously rub a comb or amber rod back and forth through a piece of fur. The comb can be tested for static charge by trying to attract a few small shreds of paper.
5. Pour some hexane from a squeeze bottle into the flow tube.
6. Place the charged comb very close to the falling stream of liquid just below the capillary opening.
7. Describe the response of the liquid in the table below.
8. Repeat the procedure with the remaining liquids.

Date _____

Name _____

Part 1: VSEPR Structures (complete at least ten from the list on the previous page)

Chemical Formula	Lewis Structure	Predicted Geometry
1. _____		_____
2. _____		_____
3. _____		_____
4. _____		_____
5. _____		_____
6. _____		_____
7. _____		_____
8. _____		_____
9. _____		_____
10. _____		_____
11. _____		_____

Name _____

Compound

Lewis Structure

1. hexane (C₆H₁₄)

Expected polarity _____

Experimental polarity _____

2. water (H₂O)

Expected polarity _____

Experimental polarity _____

3. chloroform (CHCl₃)

Expected polarity _____

Experimental polarity _____

4. acetone (CH₃-(CO)-CH₃)

Expected polarity _____

Experimental polarity _____