

Introduction to Molecules:

A Molecular Bonding and Shapes Investigation

Carolina Distance Learning

Investigation Manual

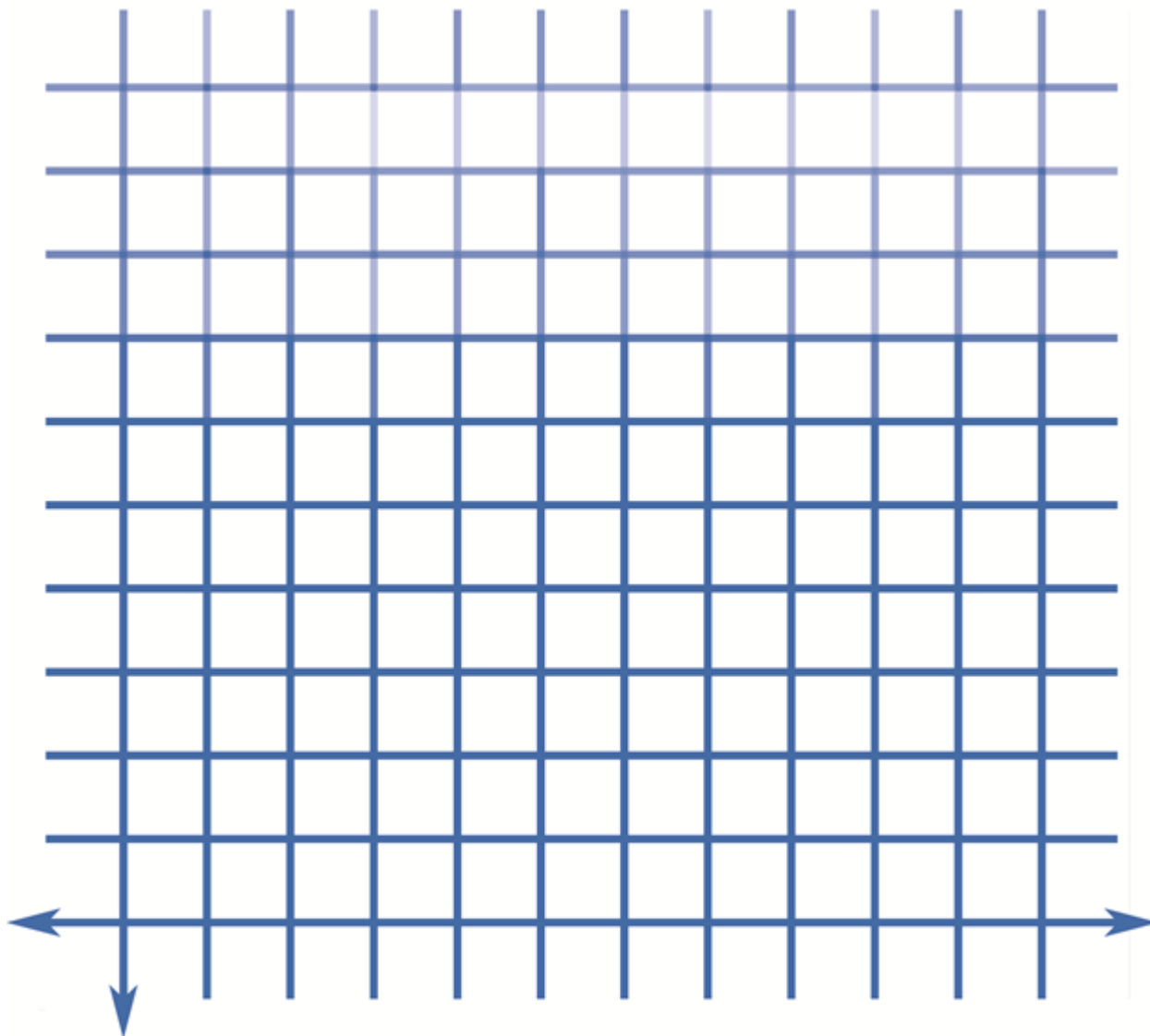


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Overview

Learn about bonding and molecular geometry using molecular models. This investigation includes classifying bonds, drawing Lewis structures, predicting molecular geometry, constructing three-dimensional models, and determining polarity. Resonance structures and isomers will also be identified as needed. The activities will require approximately 2 hours to complete.

Objectives

- Use electronegativity difference to classify bonds as ionic, polar covalent, or nonpolar covalent.
- Apply valence bond theory to draw appropriate Lewis structures.
- Apply valence shell electron pair repulsion theory (VSEPR) to predict molecular geometry.
- Construct three-dimensional molecular models.
- Sketch three-dimensional line structures using dashed lines and wedges.
- Determine whether the polarity of a molecule results in a dipole moment.
- Identify resonance structures and isomers as needed.

Time Requirements

Preparation.....	10 minutes
Activity 1: Lewis Dot Structures.....	30 minutes
Activity 2: Electron Domain Geometries	30 minutes
Activity 3: Molecular Geometry	30 minutes
Activity 4: Bonding and Polarity.....	20 minutes
Activity 5: Modeling Hydrocarbons.....	40 minutes

Background

Few elements exist in nature as single atoms. Other than the noble gases, the atoms in most elements are bonded to other atoms. This is because atoms are more stable if their outer energy level is full. Electrons in the outer energy level are called valance electrons. The halogens (Group 17 in Figure 1) have seven valance electrons in their outer energy level.

	Group 1	Group 2	Group 13	Group 14	Group 15	Group 16	Group 17	Group 18
Period 1	• H							:He:
Period 2	• Li	• Be	• B •	• C •	: N •	: O •	: F :	: Ne :
Period 3	• Na	• Mg	• Al •	• Si •	: P •	: S •	: Cl :	: Ar :
Period 4	• K	• Ca	• Ga •	• Ge •	: As •	: Se •	: Br :	: Kr :
Period 5	• Rb	• Sr	• In •	• Sn •	: Sb •	: Te •	: I :	: Xe :
Period 6	• Cs	• Ba	• Tl •	• Pb •	: Bi •	: Po •	: At :	: Rn :
Period 7	• Fr	• Ra						

Valence Electrons for the representative elements

Figure 1

Each element in group 18 has a full outer energy level. For most elements, a full outer energy level has eight electrons, or an octet. Helium and hydrogen are exceptions in that they only require two valence electrons.

Atoms can fill their outer energy level by transferring or sharing electrons to form either ionic or covalent compounds (Figure 2.)

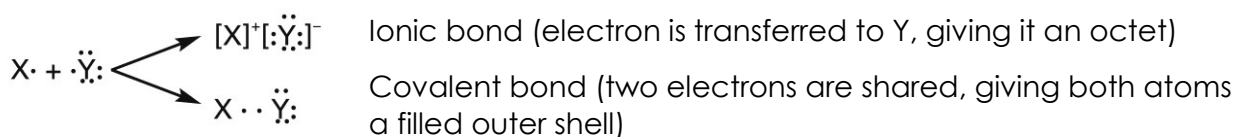


Figure 2. Ionic and Covalent Bonds

The tendency for atoms to bond ionically or covalently is determined by the difference in their electronegativity. Electronegativity is a dimensionless number that is a measure of an atom's ability to attract bonding valence electrons. Electronegativity values show periodic trends on the periodic table, as shown in Figure 3.

Periodic Table of the Electronegativities

1

H

2.1

Group 1

3

Li

1.0

Group 2

4

Be

1.5

11

Na

0.9

12

Mg

1.2

19

K

0.8

20

Ca

1.0

21

Sc

1.3

22

Ti

1.5

23

V

1.6

24

Cr

1.6

25

Mn

1.5

26

Fe

1.8

27

Co

1.8

28

Ni

1.8

29

Cu

1.9

30

Zn

1.6

31

Ga

1.6

32

Ge

1.8

33

As

2.0

34

Se

2.4

35

Br

2.8

36

Kr

3.0

37

Rb

0.8

38

Sr

1.0

39

Y

1.2

40

Zr

1.4

41

Nb

1.6

42

Mo

1.8

43

Tc

1.9

44

Ru

2.2

45

Rh

2.2

46

Pd

2.2

47

Ag

1.9

48

Cd

1.7

49

In

1.7

50

Sn

1.8

51

Sb

1.9

52

Te

2.1

53

I

2.5

54

Xe

2.6

55

Cs

0.7

56

Ba

0.9

57

La

1.1

72

Hf

1.3

73

Ta

1.5

74

W

1.7

75

Re

1.9

76

Os

2.2

77

Ir

2.2

78

Pt

2.2

79

Au

2.4

80

Hg

1.9

81

Tl

1.8

82

Pb

1.8

83

Bi

1.9

84

Po

2.0

85

At

2.2

86

Rn

2.4

87

Fr

0.7

88

Ra

0.9

89

Ac

1.1

104

Rf

105

Db

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Sg

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Bh

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Uub

5

B

2.0

6

C

2.5

7

N

3.0

8

O

3.5

9

F

4.0

10

Ne

13

Al

1.5

14

Si

1.8

15

P

2.1

16

S

2.5

17

Cl

3.0

18

Ar

19

K

0.8

20

Ca

1.0

21

Sc

1.3

22

Ti

1.5

23

V

1.6

24

Cr

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Cs

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Ca

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Sc

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Cr

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Mn

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Fe

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Co

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Ni

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29

Cu

1.9

30

Zn

1.6

31

Ga

1.6

32

Ge

1.8

33

As

2.0

34

Se

2.4

35

Br

2.8

36

Kr

3.0

37

Rb

0.8

38

Sr

1.0

Figure 3

Excluding the noble gases, the most electronegative element is fluorine, which is assigned a value of 4.0. All the other elements have calculated values based on that of fluorine. Across each period the electronegativity tends to increase, with the nonmetal families of nitrogen, oxygen, and fluorine having the highest values. This is because these atoms have smaller radii within which the positive nuclei exert a greater attraction for the valence electrons. The alkali metals and alkaline earth metals (the groups on the left side of the periodic table) have the lowest electronegativity because their atoms have the largest radii, within which the positive nuclei exert a smaller attraction for valence electrons. Cesium and francium, with the largest radii, have the lowest electronegativity value of 0.7.

Materials

Included in the materials kit:

25 balloons

Needed from the modeling kit:

Molecular model set

Needed from the equipment kit:

Ruler

Needed, but not supplied:

Calculator

Digital camera or smart phone

Pencil

Reorder Information: A replacement kit for Bonding and Molecular Geometry item number 580306, can be ordered from Carolina Biological Supply Company. Call 1-800-334-5551 to order.

Safety

Read all instructions for this laboratory activity before beginning. Follow the instructions closely and observe established laboratory safety practices, including use of appropriate personal protective equipment (PPE) as described in the Safety and Procedure section.

Model pieces can be a choking hazard. Keep these and all laboratory materials away from children.

Latex balloons are included in this kit and can cause an allergic reaction in some individuals. Individuals sensitive to latex should not participate in any activities that may result in exposure.

Preparation

1. Read the Student Guide.
2. Obtain all materials.
3. Separate model pieces into tray compartments based on shape, color, and number of prongs.

Activities 1, 3, and 4 are inter-related. The compounds used in Activity 1 are also used in Activities 3 and 4. Data in Table 1 will be used for these activities.

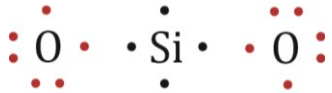
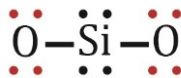
Activity 1

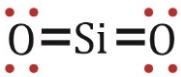
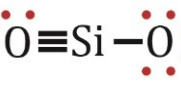
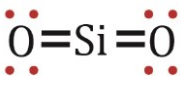
Lewis Dot Structures

A Lewis dot structure is one way to represent the arrangement of valence electrons in a molecule. In Lewis structures, each element symbol is surrounded by a specific number of dots representing valence electrons. Most atoms obey the octet rule* which states that atoms tend to combine in such a way that they each have eight electrons in their valence shells, giving them the same electronic configuration as a noble gas.

**Exceptions: Hydrogen and helium need only two valence electrons to fill their outer shell. Boron and beryllium form compounds with less than eight electrons and elements in periods 3-6 may use more than eight.*

To fill their outer shells, elements form covalent bonds by sharing electrons. Lewis structures are often used to show those bonds. Covalent compounds may have single, double, or triple bonds between atoms. These bonds are represented in a Lewis structure by dashes between the chemical symbols of the bonded elements. The number of dashes corresponds to the number of bonds. Lewis structures also indicate the lone pairs of electrons on different atoms. Guidelines for drawing a Lewis structure for a given chemical formula are as follows:

Guidelines for Drawing Lewis Structures	Example SiO ₂
1. Determine the number of valence electrons present for each atom in the compound (consult Figure 1 in the background section as needed).	Silicon (Si): 4 valence electrons Oxygen (O): 6 valence electrons Oxygen (O): 6 valence electrons
2. Find the sum of valence electrons of all the atoms. If there is a charge on a compound, add an electron for each negative charge and subtract an electron for each positive charge.	Silicon (Si): 4 valence electrons Oxygen (O): 6 valence electrons <u>Oxygen (O): 6 valence electrons</u> 16 total electrons
3. Determine which atom is to be the central atom. This is typically the least electronegative element (that is not hydrogen) and/or the first element in the chemical formula. Some compounds will have no central atom, but the first element in the formula is a good place to start.	Si
4. Write the chemical symbol of the central atom, followed by the chemical symbols for other atoms around it.	O Si O
5. Use dots to show the appropriate number of valence electrons around each symbol in the compound, based on their position in the periodic table.	
6. Determine the total number of electrons required for each element. Allow for exceptions to the octet rule as needed.	Silicon (Si) needs 8 valence electrons Oxygen (O) needs 8 valence electrons Oxygen (O) needs 8 valence electrons
7. Create a skeleton structure by connecting unpaired electrons from the central atom to unpaired electrons on the atoms around it with a solid line. Each solid line now represents a (two-electron) covalent bond between the two atoms.	
8. Redraw the structure as needed. If multiple bonds exist between two atoms, reorient the chemical symbols so that multiple bonds are with each other.	

9. Sometimes there will be more than one way to add the bonds. To determine which Lewis structure is the best model, formal charge is often used. To determine the formal charge of atoms: - Count the number of valence electrons that each atom typically has when unbound. - In the Lewis structure being evaluated, count the number of assigned electrons for an atom by counting the number of electrons that exist around that atom as lone pairs and then counting the number of covalent bonds on that atom. Add the number of lone pair electrons and the number of bonds together. - Subtract the number of assigned electrons from the number of valence electrons. The resulting value is the formal charge for the atom in that Lewis structure.	 <table style="margin: 10px auto; width: 80%;"> <tr> <td>unbound electrons</td> <td>6</td> <td>4</td> <td>6</td> </tr> <tr> <td><u>assigned electrons</u></td> <td>-6</td> <td>-4</td> <td>-6</td> </tr> <tr> <td>formal charge</td> <td>0</td> <td>0</td> <td>0</td> </tr> </table>  <table style="margin: 10px auto; width: 80%;"> <tr> <td>unbound electrons</td> <td>6</td> <td>4</td> <td>6</td> </tr> <tr> <td><u>assigned electrons</u></td> <td>-7</td> <td>-4</td> <td>-5</td> </tr> <tr> <td>formal charge</td> <td>-1</td> <td>0</td> <td>+1</td> </tr> </table>	unbound electrons	6	4	6	<u>assigned electrons</u>	-6	-4	-6	formal charge	0	0	0	unbound electrons	6	4	6	<u>assigned electrons</u>	-7	-4	-5	formal charge	-1	0	+1
unbound electrons	6	4	6																						
<u>assigned electrons</u>	-6	-4	-6																						
formal charge	0	0	0																						
unbound electrons	6	4	6																						
<u>assigned electrons</u>	-7	-4	-5																						
formal charge	-1	0	+1																						
10. Lewis structures should show negative charge on the most electronegative elements and positive charges on the least electronegative elements.	 is the preferred structure of SiO₂																								

Use the Guidelines for Drawing Lewis Structures to complete the Data Table for Activity 1.

Activity 2

Electron Domain Geometries

The three-dimensional shape of a molecule is predicted using the valence-shell electron-pair repulsion (VSEPR) model. The VSEPR model is used to predict structures of molecules or ions that contain only non-metals by minimizing the electrostatic repulsion between the regions of high electron density. In this activity, balloons will model electron domains. An electron domain is either a bond or a lone pair of electrons. Double and triple bonds count as only one domain when using the VSEPR model. When tied together, balloons naturally adopt the lowest energy arrangement predicted by the VSEPR model.

Linear Geometry – Two Electron Domains

1. Inflate a balloon and tie the open end in a knot.
2. Repeat to prepare a second balloon of approximately the same size.
3. Tie the two balloons together in a knot.
4. Label the model and photograph it for future reference.

Trigonal Planar Geometry – Three Electron Domains

1. Inflate and tie three balloons.
2. Tie the three balloons together. Start by tying two balloons together and then use the free ends to knot around the third.
3. Label the model and photograph for future reference.

Tetrahedral Geometry – Four Electron Domains

1. Inflate and tie four balloons.
2. Tie the balloons together to form two sets of two balloons.
3. Twist the two sets of two balloons together by crossing the knotted centers.
4. Label the model and photograph it for future reference.

Trigonal Bipyramidal Geometry – Five Electron Domains

1. Inflate and tie five balloons.
2. Tie four balloons together to form two sets of two balloons.
3. Tie a third balloon to one of the sets.
4. Twist the set of three balloons and the set of two balloons together by crossing the knotted centers.
5. Label the model and photograph it for future reference.

Octahedral Geometry – Six Electron Domains

1. Inflate and tie six balloons.
2. Tie the balloons together to form three sets of two balloons.
3. Twist two sets of two balloons together by crossing the knotted centers. Twist a third set of two balloons into the other two by crossing the knotted centers.
4. Label the model and photograph it for future reference.

Activity 3

Molecular Geometry

Electron Domains	No Lone Pairs	One Lone Pairs	Two Lone Pairs	Three Lone Pairs
2 <i>Geometry:</i> Bond Angles	 linear 180°			
3 <i>Geometry:</i> Bond Angles	 trigonal planar 120°	 bent <120°		
4 <i>Geometry:</i> Bond Angles	 tetrahedral 109.5°	 trigonal pyramidal 107°	 bent / angular 104.5°	
5 <i>Geometry:</i> Bond Angles	 Trigonal bipyramidal 90°, 120°	 See-saw 90°, 120°	 T-shaped 90°	 linear 180°
6 <i>Geometry:</i> Bond Angles	 octahedral 90°	 square pyramidal 90°	 square planar 90°	

- Construct a three-dimensional model of each molecule from Activity 1 using the following molecular model pieces to represent atoms.

- | | |
|--------------------------------------|---|
| a. White one-pronged: | Hydrogen |
| b. Light green one-pronged | All other atoms |
| c. Dark brown three-pronged: | Atoms with only three electron pairs and/or bonds |
| d. Black, four-pronged: | Carbon |
| e. Blue, four-pronged: | Nitrogen |
| f. Red, four-pronged: | Oxygen |
| g. Purple five-pronged: and/or bonds | Atoms with five electron pairs |
| h. Silver six-pronged: | Atoms with six electron pairs and/or bonds |

Use white tubes to connect the pronged pieces and represent covalent bonds between atoms in each molecule.

As needed, connect the white flat pieces for electron pairs on the central atom.

2. Use the white tubes to form bonds between the atoms. Each tube represents one bond (two electrons). For a double bond, use two tubes and two prongs on each atom.
3. Label each model and photograph it for future reference.
4. Sketch a perspective drawing of each compound. If necessary, use wedges and dashes to show the three-dimensional appearance using the following table:

Electron Domains	No Lone Pairs	One Lone Pairs	Two Lone Pairs	Three Lone Pairs
2	$X-A-X$			
3				
4				
5				
6				

5. Build models for all the compounds in Activity 1.

Activity 4

Bonding

Chemical bonds are shared electrons between two atoms. If the atoms are different, the attraction for these shared electrons will also be different. Chemical bonds are classified as covalent or ionic. Electrons are equally shared in non-polar covalent bonds, unequally shared in polar covalent bonds, and fully transferred to the more electronegative atom in ionic bonds.

To determine the type of bond between two atoms, first calculate the difference between their electronegativity values. Only the absolute difference is important.

Non-polar Covalent: If the difference in electronegativity is < 0.3 , the electrons are equally shared between the two atoms and the bond is a non-polar covalent bond. Some examples of molecules with non-polar covalent bonds are Cl_2 , H_2 , CH_4 , and CS_2 .

Polar Covalent: When the difference in electronegativity is between 0.4 and 1.7, there is an unequal sharing of the electrons between the two atoms. Although all electrons are constantly moving within the bonding orbital, in polar covalent bonds the electrons are more attracted to the atom with higher electronegativity and will spend more time closer to that atom. This unequal sharing creates poles of charges, thus these bonds are termed polar covalent bonds. Some examples of polar covalent molecules are NH_3 and H_2O .

Ionic: This type of bond occurs when there is complete transfer of the electrons between the two atoms. This occurs when the difference in electronegativity is > 1.8 . NaCl and MgCl_2 are typical examples.

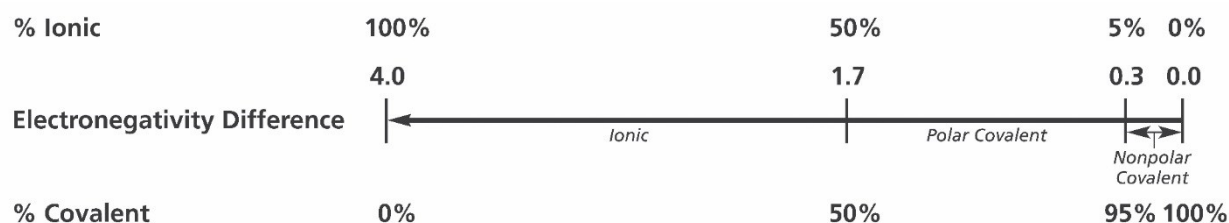


Figure 4 Bonding Scale

Sample Bond Type Calculations

Bonding Pair	Electronegativity Difference	Type of Bond
Li and F	$ 1.0 - 4.0 = 3.0$	Ionic
F and F	$ 4.0 - 4.0 = 0$	Non-polar covalent
C and F	$ 2.5 - 4.0 = 1.5$	Polar covalent

Bond Polarity

The term polar refers to the poles of partial charge. In a polar covalent bond, electrons are more attracted to the atom with greater electronegativity. This difference results in a partial negative charge on the more electronegative atom, and a partial positive charge on the less electronegative atom. Consider the compound hydrochloric acid, HCl. The electronegativity difference is 0.9 ($|3.0 - 2.1| = 0.9$). Chlorine is more electronegative than hydrogen and therefore pulls the bonding pair closer, giving the hydrogen a partial positive charge (delta plus, $\delta+$) and the chlorine a partial negative charge (delta minus, $\delta-$), as shown in Figure 5.

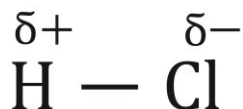


Figure 5. Hydrochloric acid, HCl, showing partial charges

Unequal sharing of electrons can also be represented by a vector indicating bond polarity. To show bond polarity, draw a vector from the positively charged atom and the negatively charged atom. Create a plus sign using a vertical line near the less electronegative atom. The vector arrow points toward the more electronegative atom, as in Figure 6.

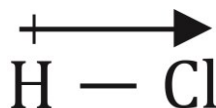


Figure 6. Hydrochloric acid, HCl, showing bond polarity

Molecular Polarity

Molecular polarity is similar to bond polarity. A polar molecule has regions of partial positive and negative charge and will orient itself in an electric field. This orientation in an electric field, called a dipole moment, is caused when charges are distributed asymmetrically within the molecule. The molecular dipole moment is shown as a vector to one side of the molecule. Once again, the vector arrow points toward the more electronegative atom, as in Figure 7.



Figure 7. Hydrochloric acid, HCl, showing molecular dipole moment

Molecules that demonstrate a dipole moment are characterized as polar. Molecules of hydrochloric acid are polar because the bond polarity is unbalanced.

Not all molecules containing polar covalent bonds are polar. If bond polarity is balanced, the partial positive and partial negative charges are distributed symmetrically. If the positive and negative charges are distributed symmetrically, the molecule does not orient itself in an electric field and does not demonstrate a dipole moment. Molecules that do not demonstrate a dipole moment are characterized as non-polar.

Magnesium chloride (Cl – Mg – Cl) is an example of a non-polar molecule that contains polar covalent bonds. Each Mg – Cl bond is polar covalent with an electronegativity difference of 0.8 (| 1.2 – 3.0 | = 0.8). However, the linear molecular geometry of magnesium chloride results in symmetrical bonds and a non-polar molecule. Magnesium chloride does not have a dipole moment because the opposing bond polarities cancel each other out (see Figure 8).



Figure 8. Magnesium chloride, MgCl₂, showing bond polarity

It is also possible to arrange polar covalent bonds symmetrically in three-dimensional space, as in carbon tetrachloride. Once again, each C – Cl bond is a polar covalent bond; the electronegativity difference is 0.5 ($|2.5 - 3.0| = 0.5$). The molecular geometry of carbon tetrachloride (tetrahedral) results in three-dimensional symmetry and a non-polar molecule. Carbon tetrachloride does not have a dipole moment because the opposing bond polarities cancel each other out (see Figure 9).

Polar molecules are always asymmetric; this can assist in identifying a molecule as polar. Polar molecules are the result of unbalanced bond polarity and therefore all polar molecules are asymmetrical in some way. If one chlorine atom in carbon tetrachloride (CCl_4) is replaced with a hydrogen atom, the molecule becomes chloroform (CHCl_3). The tetrahedral molecule is no longer symmetric; it is now both asymmetric and polar. This molecule has a region of partial positive charge near the hydrogen atom and a region of partial negative charge near the chlorine atoms. This configuration results in a molecular dipole moment shown by the large vector on the far right (see Figure 10).

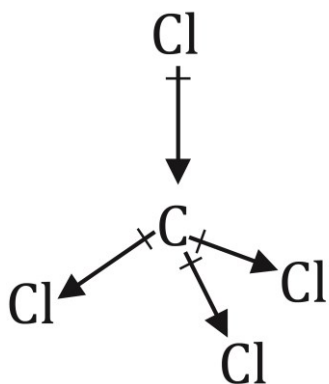


Figure 9. Carbon tetrachloride, CCl_4 , showing cancelation of polar bonds

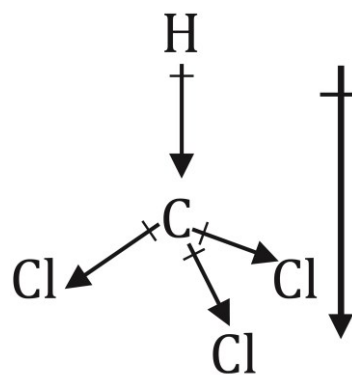


Figure 10. Chloroform, CHCl_3 , a polar molecule

The presence of lone pairs of electrons can also contribute to the polarity of a molecule. When lone pairs are present, they are regions of partial negative charge. However, not all molecules containing lone pairs are polar. The combination of molecular geometry and multiple lone pairs may result in a symmetric, non-polar molecule.

1. Complete Data Table 2 using the Periodic Table of Electronegativities and the Bonding Scale to determine the type of bond that each set of atoms would exhibit if they formed a bond. For polar covalent bonds only, draw a vector between atoms showing bond polarity in the last column.
2. Determine the electronegativity difference and bond polarity for each bond in compounds in Data Table 1. Record your calculations and bond polarity determination under Activity 4 in Data Table 1.
3. Add appropriate bond polarity vectors beside each bond in the perspective drawings under Activity 3 in Data Table 1.
4. Determine whether each molecule exhibits a dipole moment and write "yes" or "no" in the space provided under Activity 4 in Data Table 1. If the drawing is not clear, remake the model of the molecule to help visualize the shape and direction of the charges.
5. Determine whether each molecule is polar and write "polar" or "non-polar" in the space provided under Activity 4 in Data Table 1.

Activity 5

Modeling Hydrocarbons

Hydrocarbons are a large class of compounds that contain only hydrogen and carbon atoms. They present a unique structural and Lewis dot challenge because the compounds can be very large and do not have one central atom. Another challenge is that each carbon atom can bond to four different atoms and a molecule such as C_5H_{12} can have three different structural formulas (see Figure 11). The different structural formulas are called isomers.

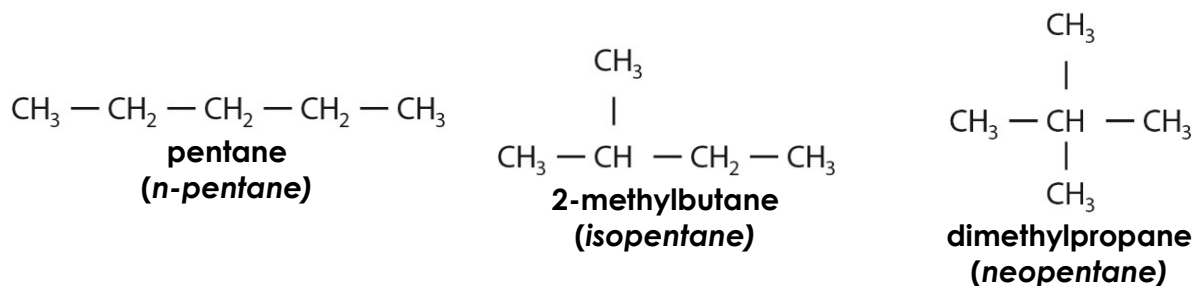


Figure 11. Different structural arrangements of pentane, C_5H_{12}

Scientists have devised numerous methods to represent molecules that do not contain a central atom. Each representation has certain advantages, as well as limitations. Commonly used representations include the molecular formula, the structural formula, the condensed structural formula, the skeletal model, the ball-and-stick model, and the space-filling model. The model or formula used depends on the information that is to be derived or conveyed. For example, to show how atoms are bonded together the structural formula might be used, but if geometry is a concern a ball-and-stick model might be preferable. The table below shows six different ways in which a pentane (C_5H_{12}) molecule can be represented.

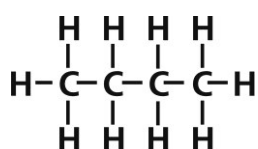
Model	Example	Advantages	Limitations
Molecular Formula	C_5H_{12}	Lists the number of atoms	Does not indicate bonding arrangements (C_5H_{12} can represent any one of three different isomers of this molecule)
Structural Formula	$ \begin{array}{ccccccccc} & H & & H & & H & & H & & H \\ & & & & & & & & & \\ H & - C & - & C & - & C & - & C & - & C & - H \\ & & & & & & & & & \\ & H & & H & & H & & H & & H \end{array} $	Shows the number of atoms and how they are bonded	Does not show the actual shape of the molecule
Condensed Structural Formula	$CH_3-CH_2-CH_2-CH_2-CH_3$ or $CH_3(CH_2)_3CH_3$	Simpler than the structural formula; shows the number of atoms and which atoms they are bonded to	Does not show the actual order bonding order
Skeletal Model		Simple model that is useful for representing large organic molecules, particularly cyclic compounds	Shows the carbon framework but not the molecule's shape; not all of the atoms and bonds are represented
Ball-and-Stick Model		Shows the number of atoms, bonding arrangements, and shape	Does not accurately show how the atoms bind
Space-Filling Model		Shows the three-dimensional shape of the molecule	The bonds are not clearly indicated. Individual atoms are difficult to see in large molecules.

Classes of Hydrocarbons

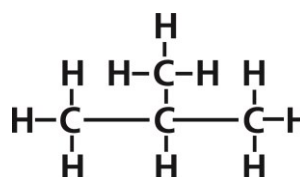
All hydrocarbons are composed entirely of carbon and hydrogen, yet their structures can vary greatly from one to the next. Hydrocarbons are categorized into five groups: alkanes, alkenes, alkynes, cyclic, and aromatic molecules.

Alkanes

Alkanes are saturated hydrocarbons because all carbon atoms are connected by single bonds. They have the general formula C_nH_{2n+2} . Alkanes can form straight chains or branched chains. All carbon atoms in an alkane adopt a tetrahedral geometry and can rotate freely in three-dimensional space. The figures below show different structural arrangements for butane, an alkane with the formula C_4H_{10} .



C_4H_{10} (n-butane)



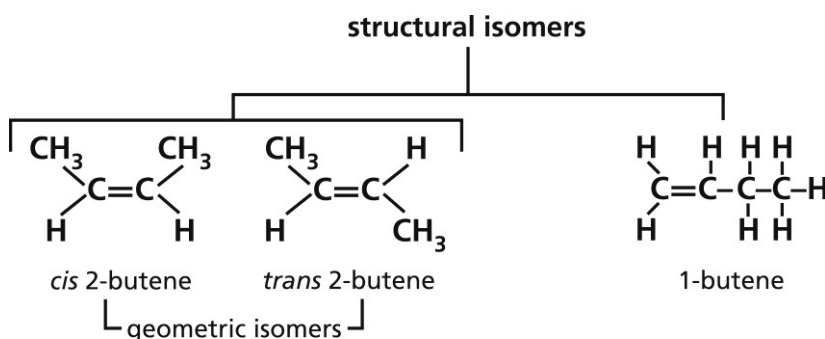
C_4H_{10} (isobutane)

Figure 12. Different structural arrangements of butane, C_4H_{10}

The first four-carbon, straight-chain molecule is normal butane, or n-butane. The second four-carbon, branched-chain molecule is isobutane (*iso-* meaning same or an isomer), or 2-methylpropane. Isobutane and n-butane are structural isomers: molecules that possess the same type and number of atoms but different bonding arrangements. Because of their structural differences, these molecules have different physical and chemical properties.

Alkenes

Alkenes are unsaturated hydrocarbons because they contain at least one double bond. Monounsaturated alkenes are characterized by the general formula C_nH_{2n} . The presence of double bonds results in carbon atoms that adopt a rigid trigonal planar geometry and cannot rotate freely. Because of these rigid bonds, alkenes can form stereoisomers in addition to structural isomers. Stereoisomers have the same bonding sequence, but the atoms are oriented differently in space. The diagram below shows three isomers of butene.



Three isomers of butene

Figure 13. Different structural arrangements of butene, C_4H_8

Because the order of its bonding arrangements is different, 1-butene is a structural isomer of *cis* 2-butene and *trans* 2-butene. However, *cis* 2-butene and *trans* 2-butene are stereoisomers, not structural isomers, because the atoms have the same bonding sequence but are oriented differently in space. When an alkene has two groups bonded to a carbon double bond on the same side, the molecule is in the *cis* position. When an alkene has two groups on opposite sides of the $C=C$ bond, the molecule is in the *trans* position. The bonds forming the $C=C$ bond are rigid,

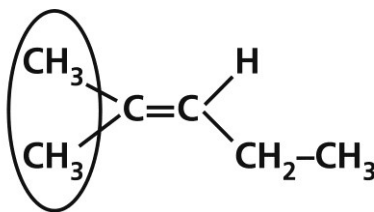


Figure 14. Molecule not exhibiting *cis-trans* isomerization

Therefore the CH_3 and H groups attached to the carbon cannot rotate to match the other carbon bond. Not all alkenes exhibit *cis-trans* isomerization. If one carbon of the double bond holds two identical groups, the molecule does not exhibit *cis-trans* isomerization.

Geometric *cis-trans* isomers are only one type of stereoisomer; hydrocarbons may also exhibit E/Z isomerization, chirality, and optical isomerization.

Alkynes

Alkynes are unsaturated hydrocarbons that contain at least one triple bond. The general formula for alkynes with one triple bond is C_nH_{2n-2} . Ethyne*, or acetylene* ($CH\equiv CH$), is the simplest of the alkynes and is shown in Figure 15. Acetylene is linear in shape, with rigid bonds that do not rotate freely. Alkynes adopt a linear shape and thus do not form geometric isomers but can form structural isomers.



Figure 15. Ethyne (acetylene), an alkyne

Ethyne is a systematic name using the suffix -yne to indicate the presence of a triple bond. In biology, ethyne is often referred to by its common name, acetylene.

Cyclic and Aromatic Hydrocarbons

In a cyclic hydrocarbon, the carbon atoms are arranged in a ring (a closed loop). The general formula for cyclic hydrocarbons is $C_nH_{2(n-g)}$, where g is the number of rings. Cyclohexane, in Figure 16, is one example of a cyclic hydrocarbon and has the formula C_6H_{12} . Alkenes can also form cyclic compounds. Cyclohexene is an example of a cyclic alkene.

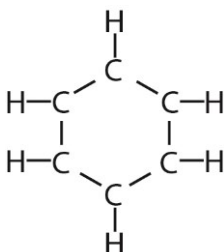


Figure 16. Cyclohexane, a cyclic hydrocarbon

Aromatic hydrocarbons are a special class of cyclic hydrocarbons. A cyclic hydrocarbon is aromatic if the carbon atoms alternate between single and double bonds. Aromatic hydrocarbons are very stable and form the backbone of many hydrocarbons. Benzene (C_6H_6) is the simplest aromatic compound, taking the form of a planar ring consisting of three double bonds and three single bonds. The figure below shows four different ways in which a benzene molecule can be represented.

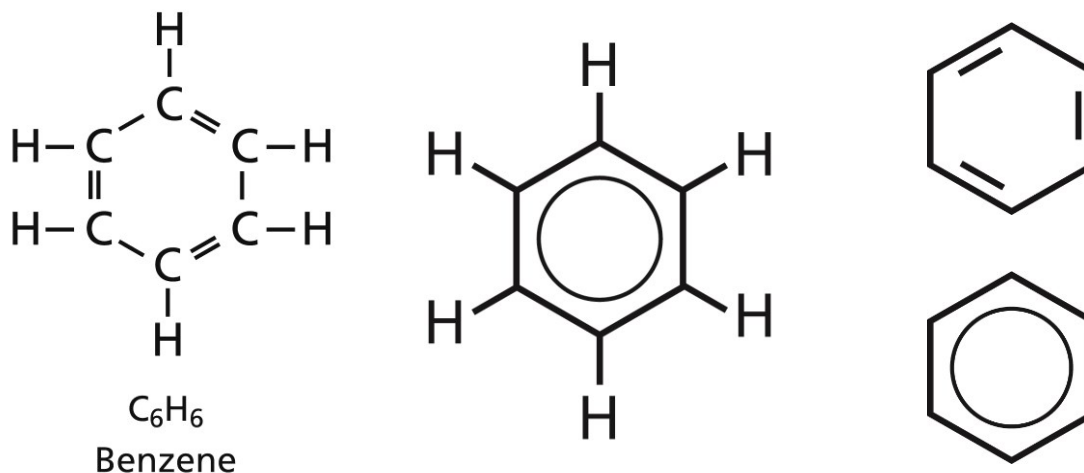
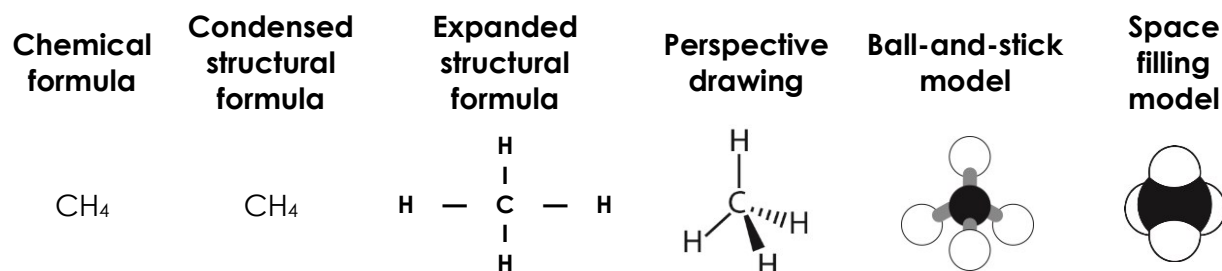


Figure 17. Four representations of a benzene molecule

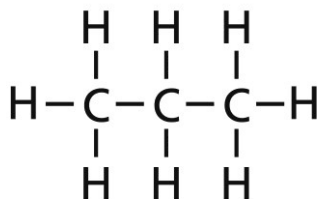
Basic Hydrocarbons

1. Form covalent bonds between a carbon and a hydrogen atom by attaching a black four-prong piece to one end of a white tube and a white one-prong piece to the other end. Throughout this activity the black pieces will represent carbon atoms and the white pieces will represent hydrogen atoms.
2. Bond hydrogen atoms to the three remaining prongs on the carbon atom.
3. This structure is a "ball-and-stick" model of the simplest hydrocarbon found in nature, a methane molecule. There are several other ways to represent this molecule.



4. Label the model as methane and photograph for future reference.

Carbon can also form single bonds with other carbon atoms to form long hydrocarbon chains. These molecules are saturated hydrocarbons because all carbon atoms are connected by single bonds. The structural formula of propane is



Propane

5. Build propane (C₃H₈) by bonding three carbon atoms together.
6. Attach a covalent bond and a hydrogen atom to all the open prongs.
7. Label the model as propane and photograph it for future reference.
8. Compare the ball and stick model that was constructed with the expanded structural formula. Describe the similarities and differences between the two representations in the Data Table.
9. Disassemble the molecular model.

Straight-Chained Hydrocarbons

- Construct molecular models of each straight chain hydrocarbon in the table below. For double and triple bonds, bend the white tubes until the required number of connections between carbon atoms has been made.

Class (bonding)	Example	General Formula	Molecular Formula	Structural Formula
Alkanes (all single C–C bonds)	ethane	C_nH_{2n+2}	C_2H_6	$ \begin{array}{c} H & H \\ & \\ H-C & -C-H \\ & \\ H & H \end{array} $
Alkenes (at least one C=C bond)	ethene	C_nH_{2n}	C_2H_4	$ \begin{array}{c} H & & H \\ & \diagdown & / \\ & C=C & \\ & / & \diagdown \\ H & & H \end{array} $
Alkynes (at least one C≡C bond)	ethyne	C_nH_{2n-2}	C_2H_2	$H-C \equiv C-H$

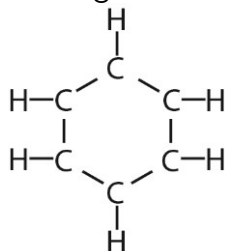
- Lay the ethane, ethene, and ethyne models side-by-side for comparison. In the Data Table, describe the following differences between the molecules:
 - Three-dimensional structure
 - Shape
 - Rotation of the bonds (i.e., can the carbon–carbon bonds rotate freely, or are they rigid?)
 - Bond strength (Which molecule has the strongest bonds?)
- Label each model and photograph them for future reference.
- Disassemble the molecular models.

Alkynes

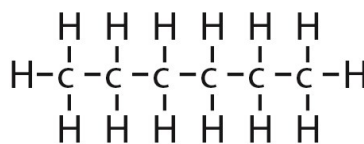
1. In the space provided on the Data Sheet, draw the structural models of all of the isomers of the alkyne C_4H_6 . Remember that alkynes contain at least one $C\equiv C$ bond.
2. Determine which structures are the same, and then eliminate the duplicates. Using the model set, build all the isomers of C_4H_6 using the structural models as reference.
3. In the space provided for observations on the Data Sheet, describe any similarities between these models and the modeled alkanes or alkenes.
4. Label each model and photograph them for future reference.
5. Disassemble the molecular models.

Cyclic and Acyclic Compounds

1. Construct a molecular model of cyclohexane and hexane using the structural models below as a guide.



Cyclohexane

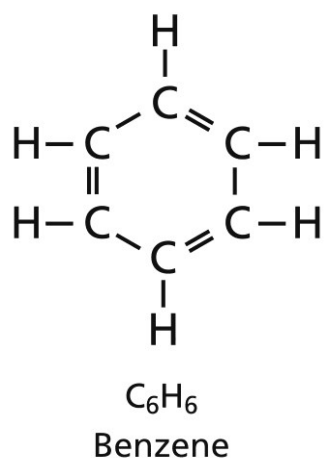


Hexane

2. Draw the skeletal model of cyclohexane and hexane on the Data Sheet.
3. Compare the structure of cyclohexane with the structure of hexane. Which arrangement is more rigid?
4. Record observations on the Data Sheet.
5. Label the models and photograph them for future reference.
6. Disassemble the molecular models.

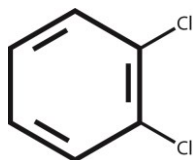
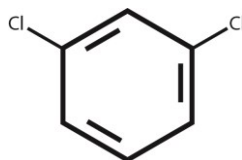
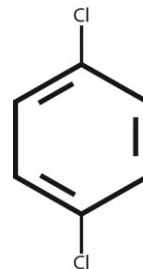
Aromatic Compounds - Benzene

1. Using the model set, build two benzene molecules using the structural models as a guide.
2. Label each model as benzene and photograph them for future reference.
3. On the Data Sheet, draw the skeletal model for both of these models of benzene.
4. Compare the two benzene models. Are these molecules isomers? Rotate both molecules and determine whether they are the same.
5. Use the two benzene models for the next activity.



Aromatic Compounds - Dichlorobenzene

1. Using the model sets from the previous activity, create the following three dichlorobenzene isomers: ortho, meta, and para.
2. One additional benzene ring will have to be made.
3. On each benzene ring, replace the hydrogen atoms with a light green one-pronged atom to represent a chlorine atom.

**Orthodichlorobenzene****Metadichlorobenzene****Paradichlorobenzene****Three isomers of dichlorobenzene**

4. Label each model with the correct name and photograph them for future reference.
5. On the Data Sheet, draw the skeletal model for both of these models of dichlorobenzene.
6. Compare the three dichlorobenzene models. Are these molecules isomers? Rotate both molecules and determine whether they are the same.
7. Can any other isomers be made with a benzene ring and two chlorine atoms?
8. Disassemble the molecular models.

Disposal and Cleanup

1. Return molecular model parts to the resealable bag for storage.

Bonding and Molecular Geometry

Choose three compounds in Group 1, three compounds in Group 2, and three compounds in Group 3 to use in Activities 1, 3, and 4. Copy each chemical formula into the spaces provided in the first column of Data Table 1.

Group 1	Group 2	Group 3
1. BeCl ₂ 2. BF ₃ 3. CH ₄ 4. PCl ₅ 5. SF ₆	6. CO ₂ 7. NH ₃ 8. H ₂ O 9. SF ₄ 10. ClF ₃ 11. XeF ₂ 12. IF ₅ 13. XeF ₄	14. O ₂ 15. HCN 16. H ₂ CO 17. CH ₃ Br 18. SnCl ₂

Data Table 1 (Make Copies of This Table)

Activity 1 Lewis Dot Structures		Activity 3 Molecular Geometry	Activity 4 Bonding and Polarity
Chemical Formula:	Central Atom:	Domains:	Electronegativity:
Dot Diagrams:	Lewis Structure:	Line Drawing:	Bond Polarity:
		Lone Pairs:	Dipole Moment:
Electrons:		Geometry:	Polarity:
		Bond Angle:	

<i>Chemical Formula:</i>	<i>Central Atom:</i>	<i>Domains:</i>	<i>Line Drawing:</i>	<i>Electronegativity:</i>
<i>Dot Diagrams:</i>	<i>Lewis Structure:</i>			
		<i>Lone Pairs:</i>		<i>Bond Polarity:</i>
		<i>Geometry:</i>		<i>Dipole Moment:</i>
<i>Electrons:</i>		<i>Bond Angle:</i>		<i>Polarity:</i>

Activity 4: Bonding and Polarity
Data Table 2

Bonding Pair	Electronegativity Difference	Type of Bond	Bond Polarity
H and H			
B and F			
Ge and F			
C and H			
N and H			
H and O			
P and Cl			
S and F			
Xe and F			
O and O			
C and O			
C and F			
Sn and Cl			
Al and O			
Na and Cl			
Mg and O			
Mg and Cl			

Activity 5: Modeling Hydrocarbons**Basic Hydrocarbons****Observation Questions:**

1. Does the ball-and-stick model look like the structural formula?
2. What differences are there between the ball-and-stick model of methane and the molecular and structural formulas above?
3. List the information that the ball-and-stick model provides that the structural and molecular formulas do not.

Straight-Chained Hydrocarbons

Class	Type of Bonding	General Formula
Alkanes		
Alkenes		
Alkynes		

Example	Structural Formula	3-Dimensional Structure	Shape	Rotation of the Bonds	Bond Strength
Ethane C ₂ H ₆					
Ethene C ₂ H ₄					
Ethyne C ₂ H ₂					

Modeling Isomers and Branched-Chain Hydrocarbons

Alkanes

Structural Isomers of C_4H_{10}

--	--

Alkenes

Isomers of C_4H_8

	Molecule 1	Molecule 2	Molecule 3
Structural Formula	$ \begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \diagdown \quad \diagup \\ \text{C} = \text{C} \\ \diagup \quad \diagdown \\ \text{H} \quad \text{H} \end{array} $	$ \begin{array}{c} \text{CH}_3 \quad \text{H} \\ \diagdown \quad \diagup \\ \text{C} = \text{C} \\ \diagup \quad \diagdown \\ \text{H} \quad \text{CH}_3 \end{array} $	$ \begin{array}{cccc} & \text{H} & \text{H} & \text{H} \\ & & & \\ \text{H} & \text{C} = \text{C} & - \text{C} & - \text{C} - \text{H} \\ & & & \\ \text{H} & \text{H} & \text{H} & \text{H} \end{array} $
Condensed Structural Formula			
Skeletal Model*			

*Skeletal models show the carbon-to-carbon bonds. Carbon atoms exist at the ends of the line segments. All hydrogen atoms and carbon-to-hydrogen bonds are understood.

Observation Questions:

1. Can Molecule 1 be made to look exactly like Molecule 2? Why or why not?
2. Describe the differences in structures between the three alkenes.
3. Are Molecule 1, Molecule 2, and Molecule 3 chemically identical?

AlkynesIsomers of C_4H_6

Observations

Cyclic and Acyclic Compounds

	Cyclohexane	Hexane
Skeletal Model		

Which arrangement is more stable, cyclohexane or hexane? Why?

Aromatic Compounds

Skeletal Models of Benzene

Are these molecules isomers or are they the same molecule? Explain.

Aromatic Compounds

Skeletal Models of Dichlorobenzene

Are these molecules isomers or are they the same molecule? Explain.