MEGA MOLECULES

Name: ____________________
Date: ____________________

Molecular Modeling Activity for Molecular Geometry

Time required: one 50-minute period

Introduction

An understanding of the structure of a molecule is fundamental to an explanation of its chemical and physical properties. For example, water is a liquid at room temperature, dissolves innumerable salts and sugars, is more dense than ice, and has a low vapor pressure, in part, because its molecules are bent rather than linear.

In this activity, you will:
(a) Construct molecular models for covalently bonded atoms in molecules
(b) Apply the valence shell electron pair repulsion theory to the geometries of molecules.

Materials

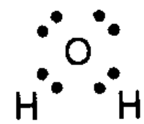
The Molecular Geometry (VSEPR) Kit

Background Information

Because structure is so important, chemists have developed a number of theories to explain and predict molecular geometries. In 1916, G. N. Lewis developed a theory that focused on the significance of valence electrons in chemical reactions and in bonding. He proposed the "octet rule," in which atoms form bonds by losing, gaining, or sharing enough electrons to have the same number of valence electrons (eight) as the nearest noble gas in the Periodic Table. The bond formed is ionic or covalent depending on whether the electrons are transferred or shared between atoms. The octet rule is valid for nearly all compounds formed between atoms of the second period and for a large number of compounds formed between atoms of other representative elements.

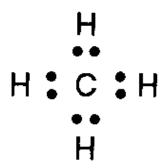
Lewis emphasized the importance of valence electrons using a Lewis symbol to represent an atom of the element—the symbol for the element surrounded with its corresponding number of valence electrons. For example, Na· is the Lewis symbol for the sodium atom, and Ca: is the Lewis symbol for calcium. The Lewis symbols for the atoms are used to account for the bonding in a compound; the resulting representation is called the Lewis formula (or Lewis structure) for the compound.

The Lewis formula for water (below) shows that by sharing valence electrons between the oxygen and hydrogen, all three atoms obtain the same number of valence electrons as the nearest noble gas; that is, the hydrogen atoms are isoelectronic with helium atoms and the oxygen atom is isoelectronic with the neon atom. Although a Lewis formula accounts for the bonding based on the valence electrons on each atom, it does not explain how the valence electrons are shared, nor does it predict any three-dimensional structure for a molecule.



VSEPR theory proposes that the geometry of a molecule is determined by the repulsive interaction of electron pairs in the valence shell of its central atom. The orientation is such that the distance between the electron pairs is maximized so that electron pair-electron pair interactions are minimized. Construction of the Lewis formula of a molecule provides the first link in predicting the geometry of the molecule.

Methane, CH_4, has four bonding electron pairs in the valence shell of its carbon atom (the central atom in the molecule).



Repulsive interactions between these four electron pairs are minimized when the electron pairs are positioned at the vertices of a tetrahedron. One can generalize that all molecules having four electron pairs in the valence shell of their central atom have a tetrahedral arrangement of these electron pairs.

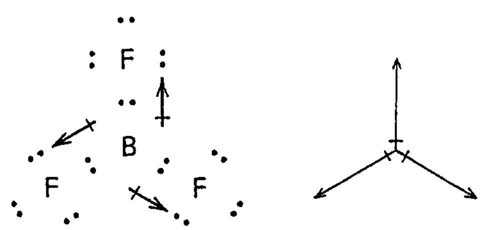
The arrangement of the bonding and nonbonding electron pairs around the central atom determines the geometric shape of the molecule.

Once the three-dimensional shape of a molecule is determined, its polarity can be qualitatively understood. A molecule is polar if an unsymmetrical distribution of electrons exists in the molecule. An unsymmetrical distribution of charge occurs when bonded atoms have different electronegativities. Table 1 lists the electronegativities of the elements. The atoms having a higher electronegativity more strongly attract bonding electrons, acquiring a greater electron density and a partial negative charge, δ^-, relative to another portion of the molecule, δ^+. The greater the electronegativity differences of the atoms, and thus the greater the distortion of the electron density, the more polar is the molecule.

The direction and magnitude of the polarity are represented by a vector, drawn in the direction of the greater electron density; the δ^+ center of the molecule is indicated by a plus sign on the tail of the vector.

If more than one polar bond exists in a molecule, the entire molecule may be polar or nonpolar, depending on the geometry of the molecule. Consider BF_3.

Using Table 2 you find that the BF_3 molecule has a VSEPR formula of AX_3. The BF_3 molecule has a trigonal planar geometry.



By comparing the electronegativities of boron and fluorine using Table 1, you find that each fluorine atom acquires a greater electron density and a partial negative charge, δ^-. The three more electronegative fluorine atoms attract the bonding electron pairs from the boron atom with equal magnitude. A geometric sum of the magnitude (all the same) and direction of the three vectors equals zero. In the BF_3 molecule no resultant vector can be drawn to indicate a resultant δ^+ or δ^- electron density in the molecule. Therefore, BF_3 is a nonpolar molecule, even though each B-F bond is polar.

Table 1: The Electronegativities of the Elements

H 2.1																	
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.1	O 3.5	F 4.1	
Na 1.0	Mg 1.3											Al 1.5	Si 1.8	P 2.1	S 2.4	Cl 2.9	
K 0.9	Ca 1.1	Sc 1.2	Ti 1.3	V 1.5	Cr 1.6	Mn 1.6	Fe 1.7	Co 1.7	Ni 1.8	Cu 1.8	Zn 1.7	Ga 1.8	Ge 2.0	As 2.2	Se 2.5	Br 2.8	
Rb 0.9	Sr 1.0	Y 1.1	Zr 1.2	Nb 1.3	Mo 1.3	Tc 1.4	Ru 1.4	Rh 1.5	Pd 1.4	Ag 1.4	Cd 1.5	In 1.5	Sn 1.7	Sb 1.8	Te 2.0	I 2.2	
Cs 0.9	Ba 0.9	La 1.1	Hf 1.2	Ta 1.4	W 1.4	Re 1.5	Os 1.5	Ir 1.6	Pt 1.5	Au 1.4	Hg 1.5	Tl 1.5	Pb 1.6	Bi 1.7	Po 1.8	At 2.0	
Fr 0.9	Ra 0.9	Ac 1.0	Lanthanides: 1.0 – 1.2 Actinides: 1.0 – 1.2														

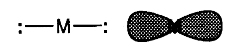
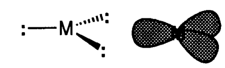
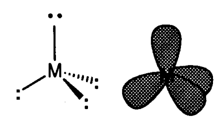
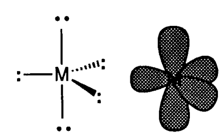
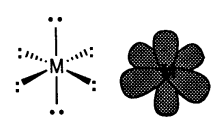
Various molecular shapes can be determined from Lewis formulas and VSEPR formulas which use the following notations:

A Refers to the central atom

X_m Refers to "m" number of bonding pairs of electrons on A

E_n Refers to "n" number of nonbonding pairs of electrons on A

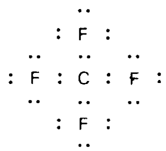
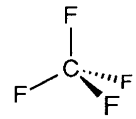
Table 2: Reference Material for Molecular Geometry

Valence Shell Electron Pairs	VSEPR Formula	Bonding Electron Pairs (VSEPR) or Bonding Orbitals (VB)	Nonbonding Electron Pairs (VSEPR) or Nonbonding Orbitals (VB)	Hybridization	Bond Angle	Geometric Shapes	Examples	Three-Dimensional Shape
2	AX_2	2	0	*sp*	180°	Linear	$HgCl_2$, $BeCl_2$	
3	AX_3	3	0	sp^2	120°	Planar triangular	BF_3, $In(CH_3)_3$	
	AX_2E	2	1	sp^2	<120°	V-shaped	$SnCl_2$, $PbBr_2$	
4	AX_4	4	0	sp^3	109.5°	Tetrahedral	CH_4, $SnCl_4$	
	AX_3E	3	1		<109.5°	Trigonal pyramidal	NH_3, PCl_3, H_3O^+	
	AX_2E_2	2	2		<109.5°	Bent	H_2O, OF_2, SCl_2	
5	AX_5	5	0	sp^3d	90°/120°	Trigonal bipyramidal	PCl_5, $NbCl_5$	
	AX_4E	4	1		>90°	Unsymmetrical Tetrahedron	SF_4, $TeCl_4$	
	AX_3E_2	3	2		<90°	T-shaped	ClF_3	
	AX_2E_3	2	3		180°	Linear	ICl_2^-, XeF_2	
6	AX_6	6	0	sp^3d^2	90°	Octahedral	SF_6	
	AX_5E	5	1		>90°	Square pyramidal	BrF_5	
	AX_4E_2	4	2		90°	Square planar	ICl_4^-, XeF_4	

Procedure

Using The Geometry of Molecules Kit of molecular models, construct the following molecules and write their Lewis formulas. Determine the number of bonding orbitals (or electron pairs involved in bonding), nonbonding orbitals (or number of nonbonding electron pairs), and degree of hybridization of the valence shell orbitals on the central atom. Also determine the VSEPR formula and the geometry of the molecule.

The central atom of the molecule is italicized. Molecules noted by an asterisk do not conform to the Lewis octet rule, even though all bonds are single bonds.

Molecule or Polyatomic Ion	Lewis Formula		Data	Sketch of the Three-Dimensional Geometry
1. CF_4		Bonding orbitals or pairs	4	
		Nonbonding orbitals or pairs	0	
		Hybridization	sp^3	
		VSEPR formula	AX_4	
		Geometry	tetrahedral	
		Polar or nonpolar	nonpolar	

Molecule	Lewis Formula	Data	Sketch of the 3-D Geometry
*BeH_2		Bonding orbitals or pairs: Nonbonding orbitals or pairs: Hybridization: **VSEPR** formula: Geometry: Polar or nonpolar:	
*BI_3		Bonding orbitals or pairs: Nonbonding orbitals or pairs: Hybridization: **VSEPR** formula: Geometry: Polar or nonpolar:	
CBr_4		Bonding orbitals or pairs: Nonbonding orbitals or pairs: Hybridization: **VSEPR** formula: Geometry: Polar or nonpolar:	
*PCl_5		Bonding orbitals or pairs: Nonbonding orbitals or pairs: Hybridization: **VSEPR** formula: Geometry: Polar or nonpolar:	

Molecule	Lewis Formula	Data	Sketch of the 3-D Geometry
*SF_6		Bonding orbitals or pairs: Nonbonding orbitals or pairs: Hybridization: **VSEPR** formula: Geometry: Polar or nonpolar:	
H_2O		Bonding orbitals or pairs: Nonbonding orbitals or pairs: Hybridization: **VSEPR** formula: Geometry: Polar or nonpolar:	
NH_3		Bonding orbitals or pairs: Nonbonding orbitals or pairs: Hybridization: **VSEPR** formula: Geometry: Polar or nonpolar:	
SiF_4		Bonding orbitals or pairs: Nonbonding orbitals or pairs: Hybridization: **VSEPR** formula: Geometry: Polar or nonpolar:	
PCl_3		Bonding orbitals or pairs: Nonbonding orbitals or pairs: Hybridization: **VSEPR** formula: Geometry: Polar or nonpolar:	
*SF_4		Bonding orbitals or pairs: Nonbonding orbitals or pairs: Hybridization: **VSEPR** formula: Geometry: Polar or nonpolar:	