STRUCTURE OF MOLECULES (VSEPR)

VALENCE SHELL ELECTRON –PAIR REPULSION (VSEPR) THEORY AND MOLECULAR MODELING

Pre-Lab Questions

1. **Draw the Lewis Electron Dot Formula for formaldehyde (H_2CO).**
2. **Which one is the central atom?**
3. **What is the steric number?**
4. **How many bonding pairs of electrons are there around the central atom?**
5. **How many non-bonding pairs of electrons are around the central atom?**
6. **What is the electronic geometry?**
7. **What is the molecular shape?**
8. **Is the compound polar?**
9. **Why is the H-O-H bond angle in a water molecule (H_2O) smaller than the H-C-H bond angles in methane (CH_4)?**

Part I. VSEPR theory and Molecular Modeling with Ball-and-Stick Models

Objective

To predict the structure and simple properties (such as polarity) of a molecule based on its Lewis Electron Dot formula and the Valence Shell Electron –Pair Repulsion (VSEPR) Theory.

Introduction to the Experiment

Many physical and chemical properties of a molecule depend on (1) the kinds of atoms that constitute it and the types of bonds that bind the atoms, and (2) the way the atoms are arranged in space, namely, the shape of the molecule (the 3-D structure of the molecule). Therefore, the structural study of a chemical species (molecule, ion) is a very important field. Chemists can predict the shapes of many molecules once a molecular formula is given. This can be done by drawing a Lewis Electron Dot Formula of a given molecule, then applying the Valence Shell Electron-Pair Repulsion Theory. The VSEPR theory states *"Electron pairs in a valence shell of an atom repel other electron pairs, and they keep apart by making the angles between them as large as possible*." Namely, the electrons will adopt an arrangement to minimize repulsion among them. Refer to Figure 1. In general, the following types of molecular shapes will occur based on the number of electron pairs around the central atom and the number atoms that are bonded to the central atom.

CLASSIFICATION OF SIMPLE MOLECULES/IONS And THEIR SHAPES:

		Examples:
(1) AB Type :	*always linear*	HCl, CO, OH^-
(2) AB_2 Type :	*linear or bent*	CO_2, H_2O, SO_2.
(3) AB_3 Type :	*planar or pyramidal*	SO_3, CO_3^{2-}, NH_3.
(4) AB_4 Type :	*planar, tetrahedral or other*	CH_4, XeF_4, SCl_4.
(5) AB_5 Type :	*Pyramidal or bipyramidal*	PCl_5, IF_5
(6) AB_6 Type :	*octahedral*	SF_6, $SnCl_6^{2-}$

Safety

No hazardous chemicals are used in this lab.

Procedure

HOW TO PREDICT 3-D STRUCTURES OF MOLECULES /IONS ?

Step 1: Write down the molecular formula.

Step 2: Draw a Lewis Electron Dot Formula, then determine the # of sets of e^- pairs around a central atom (this is called a steric number or number of areas of electron density).

Step 3: Place the electronic sets around the central atom so that they keep as far away as possible from each other applying the VSEPR Theory.

Step 4: Attach surrounding atoms to the bonding electron pairs in the central atom to have a particular 3-D structure. (See the Summary below.)

Step 5: Determine symmetry of the molecule.

Step 6: Determine polarity: Polar if asymmetrical. Non-Polar if symmetrical.

Step 7: Predict the properties of the molecule/ion.

number of electron sets	Electronic Geometry
2	Line
3	Trigonal Planer
4	Tetrahedron
5	Trigonal Bipyramid
6	Octahedron

Summary of Molecular Structures and Polarity from the VSEPR Theory

Steric number	Electronic Geometry (Orbital Type)	Bonding Pairs	Molecular Shape	Point of Symmetry?	Polar Y/N)	Examples
2	Line (sp)	2	Line	Yes	No	$BeCl_2$
3	Trigonal (sp2)	2	Bent	No	Yes	SO_2
		3	Trigonal	Yes	No	BF_3
4	Tetrahedron (sp3)	1	Line	No	Yes	HF
		2	Bent	No	Yes	SCl_2
		3	Trigonal pyramid	No	Yes	PCl_3, H_3O^+
		4	Tetrahedron	Yes	No	$CHCl_3$
5	Trigonal bipyramid	2	Linear	Yes	No	XeF_2
	(sp^3d)	3	T-shape	No	Yes	ClF_3
		4	Seesaw	No	Yes	SF_4
		5	Trigonal bipyramid	Yes	No	PF_5
6	Octahedron	4	Square	Yes	No	XeF_4
	(sp^3d^2)	5	Square pyramid	No	Yes	BrF_5
		6	Octahedron	Yes	No	SeF_6

LABORATORY EXERCISE

For the given molecules,

(1) Draw the Lewis electron dot formula. The least electronegative atom should be placed at the center of the molecule (The H atom is an exception. It must always be at a terminal position.)

(2) Find the number (steric #) of bonding pairs of electrons and the number of non-bonding pairs of electron around the central atom. Build the electronic model with a ball and sticks.

(3) First, apply the VSEPR Theory to determine its electronic geometry.

number of electron sets	Electronic Geometry	Orbital Types
2	Line	sp
3	Trigonal Plane	sp^2
4	Tetrahedron	sp^3
5	Trigonal Bipyramid	sp^3d
6	Octahedron	sp^3d^2

(4) Add surrounding atoms to the bonding electron pairs in the central atom to have a particular3-D structure (molecular geometry). Use the balls in the model kit to attach the surrounding atoms to the electronic sticks accordingly.

(5) Determine the symmetry of the molecule.

(6) Determine the polarity of the molecule: Polar if asymmetrical. Non-Polar if symmetrical. Next, predict its simple properties such as the strength of intermolecular forces.

(7) (Optional) If a molecular modeling program (such as Spartan, HyperChem) is available,
Build the structure with the software for water (H_2O), ammonia (NH_3), methane (CH_4) to confirm your structure, then try to find out bond lengths and bond angles in each of the molecules.

An Exercise with Ammonia, NH_3

(1) In the Lewis Electron Dot Formula, the N atom must be placed at the center with 4 pairs of electrons around it. Each of the three H atoms is bonded with a pair of electrons (single bond) to oxygen. One pair of electron is not used in the bonding.
(2) The electron dot formula yields four electron dense regions. Namely, the steric # is four: three bonding pairs and one non-bonding pair.
(3) The VSEPR forces the four electronic groups be place at the corner of a **tetrahedron.** Namely, it generates an electronic geometry of tetrahedron.
(4) Since there are only three terminal H are available, the molecular geometry becomes a **trigonal pyramid**.
(5) This molecule is not symmetrical with respect to a point.
(6) Therefore, it is a polar.
(7) Since N is very electronegative and it is polar, one can predict that ammonia exhibits a moderate intermolecular force, a lower vapor pressure, and relatively high boiling point.

The Molecules for Lab Exercise:

	Lewis Formula	Central Atom	Steric Number	Electronic Geometry	Number of Bonding Pairs	Number of Lone Pairs	Molecular Shape	Polar ? (Y/N)
(A) CO_2	*(O=C=O)*	*C*	*2*	*Linear*	*2*	*0*	*Linear*	*No*
(B) SO_2								
(C) SO_3								
(D) HCl								
(E) H_2O								
(F) H_3O^+								
(G) CH_4								

	Lewis Formula	Central Atom	Steric Number	Electronic Geometry	Number of Bonding Pairs	Number of Lone Pairs	Molecular Shape	Polar ? (Y/N)
(H) NH_4^+								
(I) XeF_2								
(J) ClF_3								
(K) SCl_4								
(L) PCl_5								
(M) XeF_4								
(N) IF_5								
(O) SF_6								
(P) $SnCl_6^{2-}$								