Molecular Models and Dipoles

Suggested reading: *Chang* text – pages 386 – 400

Purpose

The purpose of this experiment is to draw the Lewis structure for selected molecules and ions and to use valence shell electron repulsion (VSEPR) theory to investigate the structural geometry of the molecules and ions.

Introduction

The chemical and physical properties of molecules and ions are directly related to the geometry of the species. The spatial arrangement of atoms and electrons in a chemical species will affect the function and reactivity of the species. Understanding the geometrical structure of chemical species gives insight into studying chemical reactivity and reaction rates. The **Lewis structure** of a species shows the spatial orientation of atoms, bonding electrons, and non-bonding electrons. There are a few standard rules used to write the Lewis structure of a species, and a useful version of the rules is given in the outline below:

Drawing Lewis Structures

1. Add up number of valence electrons.
   a. # valence electrons = group number
   b. adjust for charge (for negative charge, add electrons ~ for positive charge, remove electrons)
2. Place least electronegative atoms in the center, most electronegative atoms (and hydrogen) on the outside.
3. Place one pair of electrons between bonded atoms
4. Use remaining electrons as lone pairs on outside atoms so all have 8 electrons surrounding them.
5. If the central atom has ***less*** than 8 electrons, make double or triple bonds using lone pairs on the outside atoms.
6. If ***extra*** electrons remain, place them on the central atom (expanded octet).
7. If there is more than one way to draw the structure with octets on all required atoms, then there are resonance forms.

Many times there is more than one acceptable Lewis structure for a species. The most plausible Lewis structure is chosen based on **formal charge analysis**. The formal charge of an atom is equal to the number of valence electrons in an isolated atom (obtained from the group number on the periodic table for Group A metals) minus the number of electrons assigned to the atom in the Lewis structure. In order to assign the number of electrons to an atom in the Lewis structure, the following rules can be used: (1) Non-bonding or lone electrons are assigned to the individual atom. (2) Each atom of a bond is assigned one-half the number of electrons contained in the bond.

A Lewis structure in which there is no formal charges (equal to zero) is preferable to one in which formal charges are present. Also, Lewis structures with large formal charges (± 2, ± 3) are less plausible than those with small formal charges (± 1). The most plausible Lewis structure is the one with small formal charges on all atoms and negative formal charges placed on the more electronegative atoms. Another convenience of formal charge analysis is that the sum of the formal charges of each atom in a species should equal the charge on the species.

The Lewis structure can be used to predict the three-dimensional shape of the species if one assumes that electrons in the valence shell of an atom repel one another. **Valence shell electron pair repulsion** (VSEPR) theory gives

Molecular Models and Dipoles

a model for predicting the three-dimensional shapes of a species. Use Table 1 on pages 5 and 6 as a guide for using VSEPR model to predict the molecular geometry of selected chemical species.

Data Sheet

Name: ______________________________________

Part A:

There exist three possible **isomers** (species having the same chemical formula but different structures) for the complex ion of OCN^{1-}. Each isomer has a different central atom (OCN^{1-}, CON^{-1}, and CNO^{1-}). Draw the possible resonance structures for each isomer and determine the most stable Lewis structure for each of the three isomers. Which of these 3 isomers is the most stable according to formal charge analysis? Explain your answer.

Molecular Models and Dipoles

Part B:

Obtain a model kit to build models and complete A – D for each molecule or ion (1) – (10) below.

A) Draw the best Lewis structure.

B) Identify the electron arrangement and molecular geometry (See Table 1 and Chapter 10 of your text book for additional information).

C) Sketch the VSEPR structure or the shape of the molecule.

D) Excluding the ions, indicate whether each molecule is polar or non-polar. Show the net dipole moment on the VSEPR sketch if polar.

(1) PO_3^{3-} Electron arrangement ____________________ Molecular Geometry ____________________ Dipole Moment **N/A**	(2) PH_3 Electron arrangement ____________________ Molecular Geometry ____________________ Dipole Moment (Circle One) YES NO
(3) CO_3^{2-} Electron arrangement ____________________ Molecular Geometry ____________________ Dipole Moment **N/A**	(4) CH_2F_2 Electron arrangement ____________________ Molecular Geometry ____________________ Dipole Moment (Circle One) YES NO

Molecular Models and Dipoles

(5) SO_2

Electron arrangement ____________________________________

Molecular Geometry _____________________________________

Dipole Moment (Circle One) YES NO

(6) $ICl_2Br_2^{1-}$

Electron arrangement ____

Molecular Geometry ____

Dipole Moment **N/A**

(7) ICl_3

Electron arrangement ____________________________________

Molecular Geometry _____________________________________

Dipole Moment (Circle One) YES NO

(8) SOF_4

Electron arrangement ____

Molecular Geometry ____

Dipole Moment (Circle One) YES NO

(9) HCN

Electron arrangement ____________________________________

Molecular Geometry _____________________________________

Dipole Moment (Circle One) YES NO

(10) CO_2

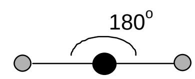
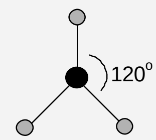
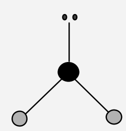
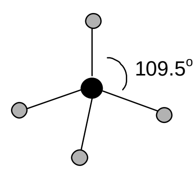
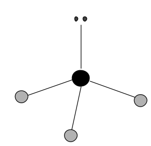
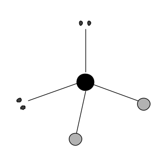
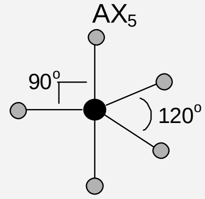
Electron arrangement ____

Molecular Geometry ____

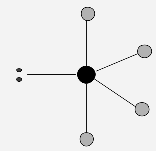
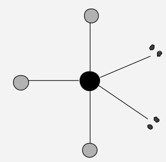
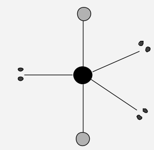
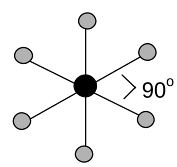
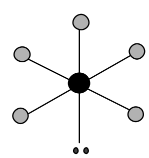
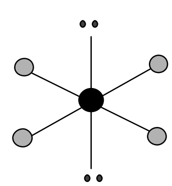
Dipole Moment (Circle One) YES NO

Molecular Models and Dipoles

Table 1: Molecular Geometry based on VSEPR Model

Total number of electron pairs around central atom (A)	Bonding pairs (X)	Non-bonding pairs (E)	Shape	Molecular Geometry
2	2	0	AX_2 	Linear
3	3	0	AX_3 	Trigonal Planar
3	2	1	AX_2E 	Bent
4	4	0	AX_4 	Tetrahedral
4	3	1	AX_3E 	Trigonal Pyramidal
4	2	2	AX_2E_2 	Bent
5	5	0	AX_5 	Trigonal Bipyramidal

Molecular Models and Dipoles

5	4	1	AX_4E 	Seesaw
5	3	2	AX_3E_2 	T-shaped
5	2	3	AX_2E_3 	Linear
6	6	0	AX_6 	Octahedral
6	5	1	AX_5E 	Square Pyramidal
6	4	2	AX_4E_2 	Square Planar