EXPERIMENT30A3: LEWIS STRUCTURES & SHAPES OF MOLECULES AND IONS

Learning Outcomes

Upon completion of this lab, the student will be able to:

1) Construct Lewis structures for simple ions and molecules.
2) Predict the shapes of simple ions and molecules from their Lewis structures.

Introduction

Lewis structures or electron dot formulas are a diagrammatic representation of the various electron groups, both bonding and non-bonding, around a central atom of an ion or molecule. Lewis structures enable the prediction of the three dimensional arrangement of the electron groups based on the **Valence Shell Electron Pair Repulsion (VSEPR)** theory.

Lewis structures can be constructed from the formula of an ion or a molecule by following a set of rules described below:

1. Count the total number of valence electrons. Add one electron for each negative charge and subtract one electron for each positive charge.

2. Place the least electronegative atom that is not hydrogen in the center.

3. Place all the other atoms around the central atom.

4. Connect the central atom to each outer atom by using a single covalent bond.

5. Complete the octet for the more electronegative outer atoms (only two electrons are required for hydrogen, four for beryllium, and six for boron).

6. Place any remaining electrons on the central atom.

7. If all the atoms do not have an octet then borrow electrons from an outer atom and construct a double or triple bond between the outer atom and the central atom.

8. Step 7 may result in multiple possibilities, called resonance structures. In case multiple possibilities exist, then find the formal charge of each atom in the structure.

    a. The structure with the lowest set of formal charges (closest to zero) is the best Lewis structure.

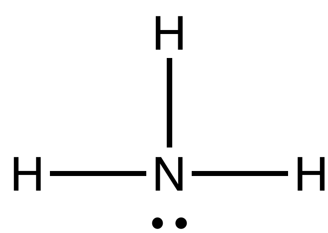
b. For structures with equal amounts of charge separation, the best structure will be the one where the negative charge is on the more electronegative atom.

9. There are a few exceptions to the octet rule:

    a. Hydrogen, beryllium, and boron, as already discussed do not complete their octet.
    b. Some nitrogen containing ions and molecules may have an odd number of total electrons and will therefore have one element with an incomplete octet.
    c. Elements in period 3 and below are able to expand their octet and accommodate more than eight electrons in their valence shells due to the availability of vacant d-orbitals.

AXE Notation

Once the Lewis structure for an ion or molecule has been constructed, a molecule or ion “type” can be assigned to the structure that will indicate the numbers of bonding and non-bonding electron groups around the central atom. For instance, consider NH_3. The Lewis structure for this molecule is shown below:



In this structure nitrogen is the central atom and hydrogen is the outer atom. There are three bonds total between the nitrogen and the hydrogen- implying there are three bonding electron groups. There is also one lone pair of electron on the nitrogen- implying there is one non-bonding electron group.

To classify ions or molecules to a type, the central atom is depicted as A, the outer atoms in the bonding group as X and the non-bonding electron group as E. Since there are three bonding groups (so, 3 of X) and one non-bonding group (so, 1 of E), NH_3 would be classified as being the type AX_3E_1. Once the type has been assigned, the following table can be used to determine the electron group geometry and the molecular geometry of the structure.

TABLE 1

Molecule or Ion type	**Total number of electron groups**	**Number of bonding electron groups**	**Number of non-bonding electron groups**	**Electron group geometry**	**Molecular geometry**	**Bond angle**
AX_2	2	2	0	Linear	Linear	180°
AX_3	3	3	0	Trigonal planar	Trigonal planar	120°
AX_2E_1	3	2	1	Trigonal planar	Bent	
AX_4	4	4	0	Tetrahedral	Tetrahedral	109.5°
AX_3E_1	4	3	1	Tetrahedral	Trigonal pyramid	
AX_2E_2	4	2	2	Tetrahedral	Bent	
AX_5	5	5	0	Trigonal bipyramidal	Trigonal bipyramidal	180°, 120°
AX_4E_1	5	4	1	Trigonal bipyramidal	See-saw	
AX_3E_2	5	3	2	Trigonal bipyramidal	T-shape	
AX_2E_3	5	2	3	Trigonal bipyramidal	Linear	
AX_6	6	6	0	Octahedral	Octahedral	90°
AX_5E_1	6	5	1	Octahedral	Square pyramid	
AX_4E_2	6	4	2	Octahedral	Square planar	

NOTE: Structures with a) lone pairs on the central atom b) double bonds will tend to have compressed bond angles.

Experimental Design

Using a molecular model kit construct the three-dimensional arrangement of the atoms of the list of molecules or ions provided below in Table 2.

TABLE 2

HCN	BeF_2	SO_2	O_3	OF_2
BF_3	CO_3^{2-}	CH_4	ClO_4^-	PF_3
H_2O	PF_5	SF_4	BrF_3	XeF_2
IOF_5	TeF_5^-	XeF_4	XeO_2F_2	SO_4^{2-}

Reagents and Supplies

Molecular model kit

Procedure

1. Draw the Lewis structure of each molecule or ion in the list above.
2. Assign the Lewis structure to a specific type.
3. Determine the electron group geometry and the molecular geometry, using Table 1.
4. Using the molecular model kit, construct the model of each structure in Table 2.
5. Also indicate the bond angles and polarity of each structure.