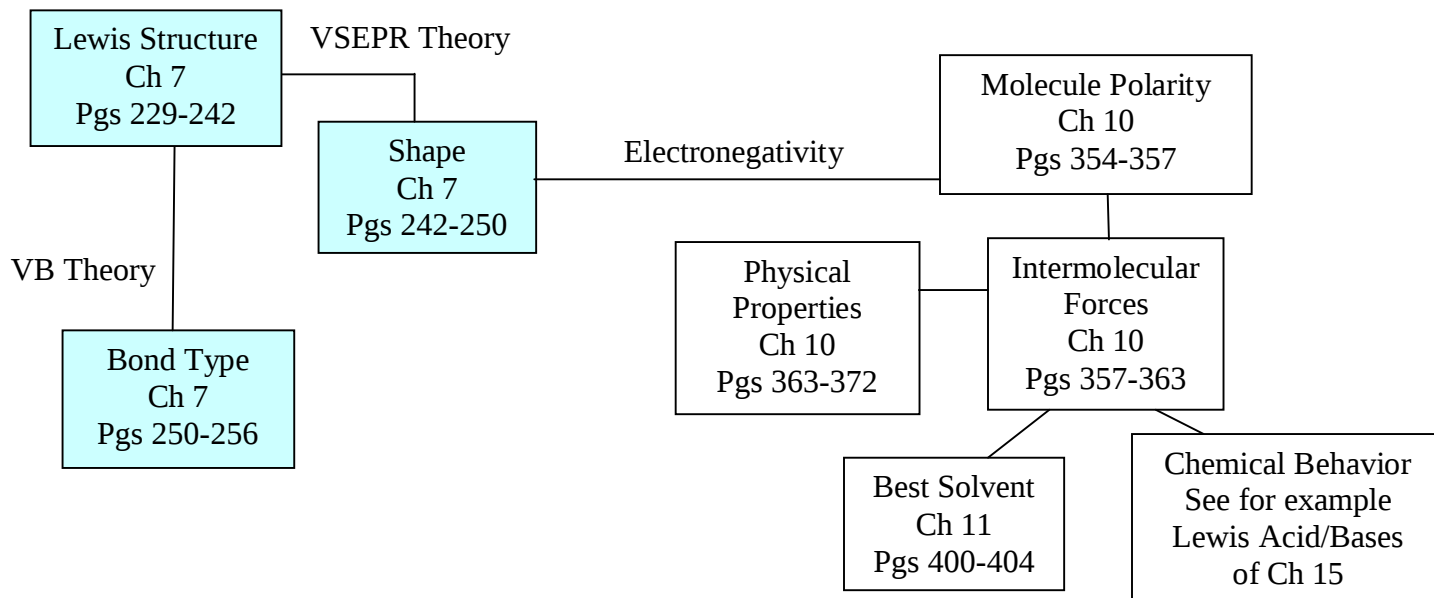


Objectives: Following this lab you should be able to draw the Lewis structure of a molecule, determine its shape using Valence Shell Electron Pair Repulsion (VSEPR) Theory, draw the molecule with the correct shape, and determine the types of bonds that are present using Valence Bond (VB) Theory.

It is an essential part of chemistry that you understand the structure of molecules and ions. You are a three dimensional object because you are made of molecules with 3-D shapes. The shape of molecules can be determined using VSEPR Theory. Before VSEPR Theory can be applied all valence electrons of the molecule must be distributed to form the Lewis Structure and bonding must be determined. Why is the shape of the molecule important? The following flow chart illustrates the importance of molecular shape to chemistry.



The first portion of the flow chart (highlighted in blue) will be described in College Chemistry I and practiced in this laboratory. The second part of this flow chart will be discussed early in College Chemistry II. Note that everything begins with the Lewis Structure.

Steps for Determining the Lewis Structure (Chapter 7, pgs 229-242)

1. Add up your total valence electrons.
2. Determine placement of the atoms. Place all other elements in the formula around the central atom.

Note:

- a. The least electronegative atom is the central atom unless that element is hydrogen. Hydrogen can never be a central atom.
 - b. Often it is the first element listed in a formula unless, again, that element is hydrogen.
3. Draw a single bond between the central atom and each of the external atoms. Subtract 2 electrons for each bond you drew from the total in Step 1.
 4. Place the remaining electrons around the external atoms until the external atoms achieve an octet. Subtract the number placed from those remaining in step 3.

Note:

- Hydrogen only needs 2 electrons to be like Helium instead of an octet.
- Boron belongs to an electron deficient family and often only needs 6 electrons.
- A free radical will typically only have 7 electrons.
- All other atoms should have a minimum of 8 to achieve an octet.

5. If there are valence electrons still to distribute after Step 4, place the electrons on the central atom in pairs until all are used up.
6. **Do all of the atoms have an octet? (If any have not satisfied the octet rule, it is typically the central atom.)**
 - a. No....then move a lone pair of electrons on a terminal atom in to form a multiple bond with the central atom.

Yes

 - i. If the central atom is in period 2, you are done.
 - ii. If the central atom is in period 3 or greater you must calculate the formal charge on the atoms to determine whether additional bonds should be made.
7. **If you alter the structure in step 6, you must repeat step 6 until no further alterations occur.**

Formal Charge (F.C.) Calculations: (Chapter 7, pgs 240-242)

The formal charge of each atom in a molecule should be calculated if the central atom is in periods 3-7. Formal charge is associated with a single atom of an element. Each atom within a molecule will have its own formal charge.

$$\text{Formal charge} = \# \text{ valence } e^- - [1 \text{ for every lone electron} + 1 \text{ for every bond}]$$

What does the formal charge of the atoms indicate? It indicates whether multiple bonds should be made between an external atom and the central atom. It also indicates the location of a charge in ions.

When should multiple bonds be made? Multiple bonds often, though not always, should be made if the formation of those bonds reduces the absolute value of formal charge throughout the molecule.

When do you know that you have arrived at the best structure?

- a. You will minimize the absolute value of the molecule's formal charge.
- b. You will not have two negative charges or two positive charges on adjacent atoms.
- c. If negative formal charges still exist in the final structure, the charge resides on the most electronegative atom.

Thus far the rules given above apply to all molecules. There are two additional concepts associated with Lewis Structures that must be covered before moving onto molecular shape. Those two items are the treatment of ions and the development of resonance structures.

Treatment of ions:

There are two key differences in the treatment of ions compared to neutral molecules. (1) You must take the charge into account when determining the number of valence electrons of a molecule. If the charge is positive, then subtract the number of electrons indicated by the charge from the total valence electrons in step 1. If the charge is negative, then add the number of electrons indicated by the charge to the total valence electrons in step 1. (2) When you have completed the Lewis structure you must indicate that the structure is that of an ion instead of a neutral molecule. To do so, you place the Lewis structure in brackets with the charge as a superscript to the right of the bracket.

Resonance Structures: (Chapter 7, pgs 238-240)

Resonance structures arise when more than one equivalent Lewis structure can be drawn for the same molecule. In reality neither Lewis structure is correct on its own. Instead the real structure is an average of valid resonance structures. How do you know when you need to draw resonance structures? A set of resonance structures will be required when you share a pair of electrons between an external atom and the central atom, but an equivalent atom could just as easily have shared electrons with the central atom.

Valence Shell Electron Pair Repulsion Theory (VSEPR Theory) (Chapter 7, pgs 242-250)

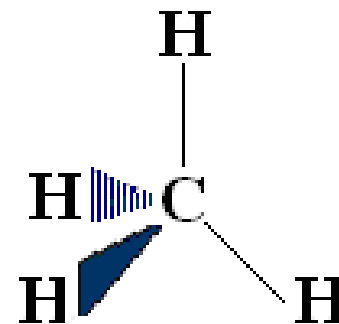
VSEPR Theory will allow for the determination of the molecular shape now that the Lewis structure of a molecule has been developed. VSEPR Theory describes the shape of the structure that arises around the **central atom**. To determine the shape you must break down the electrons surrounding the central atom into bonding groups and non-bonding groups. A single bond, a double bond, and a triple bond attached to the central atom are all defined as a single bonding group. Pairs of electrons or a lone electron, in the case of a free radical, are defined as a single non-bonding group.

Important Facts:

1. VSEPR theory – valence shell electrons surrounding the central atom will repel each other so that they are as far apart as possible. The basic geometry is therefore determined by the # of electron groups surrounding the central atom.
2. Although the basic geometry is determined by all of the electron groups surrounding the central atom of the molecule the shape describes only the bonding groups surrounding the central atom.
3. The ideal bond angle is only valid if all atoms and bond types surrounding the central atom are the same. If the bond types or groups surrounding the central atom vary then the bond angles will change
4. Spatial requirements: Lone pairs take up more space than do bonding groups because the electrons are attached to a single atomic nucleus and are therefore allowed to spread out more. This causes a reduction in angle for the remaining bonds.
5. To draw the molecules correctly simply substitute the outer circles with your outer atoms and the inner circles with your central atom.

Chemists use universal notation to draw a 3-D molecule on paper. This notation allows the reader to understand whether a bond lies within the same plane as the central atom, whether the bond extends out of the front of the paper toward the reader, or whether the bond extends behind the paper away from the reader.

- A straight line (—) indicates that the bond lies in the same plane as the central atom.
- A darkened in wedge () indicates that the bond extends out the front of the paper, towards the reader.
- A dashed wedge () indicates that the bond extends out the back of the paper, away from the reader.



The following table illustrates how the # of bonding groups and the # of non-bonding groups determine the shape of the molecule.

Geometry and Bonding: Data Sheet

sulfur dichloride, SCl_2

valence electrons:

Lewis structure:

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

hydronium ion, H_3O^+

valence electrons:

Lewis structure (indicate formal charges):

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

arsenic trichloride, AsCl₃

valence electrons:

Lewis structure:

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

hydrogen peroxide, H₂O₂

valence electrons:

Lewis structure (indicate formal charges):

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

carbon dioxide, CO₂

valence electrons:

Lewis structure:

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

sulfur dioxide, SO₂

valence electrons:

Lewis structure (indicate formal charges):

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

carbonate, CO₃²⁻

valence electrons:

Lewis structure:

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

nitrogen dioxide, NO₂

valence electrons:

Lewis structure (indicate formal charges):

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

arsenic trichloride, AsCl₃

valence electrons:

Lewis structure:

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

hexafluorophosphate ion, PF₆⁻

valence electrons:

Lewis structure (indicate formal charges):

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

selenium tetrafluoride, SeF₄

valence electrons:

Lewis structure:

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

tribromide ion, Br₃⁻

valence electrons:

Lewis structure (indicate formal charges):

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

xenon tetrafluoride, XeF₄

valence electrons:

Lewis structure:

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

iodine pentafluoride, IF₅

valence electrons:

Lewis structure (indicate formal charges):

Geometry description:

Hybridization of central atom;

Bonding description:

Draw the molecule with the correct shape.

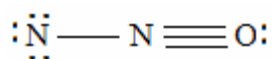
Geometry and Bonding: Pre-laboratory Assignment

1. Consider the compound sodium nitrate.

(a) What types of bonding are present in this compound?

(b) Provide a clear dot structure representation of sodium nitrate demonstrating the types of bonding identified in (a).

2. Several different Lewis dot structures can be drawn for the dinitrogen monoxide molecule. One is



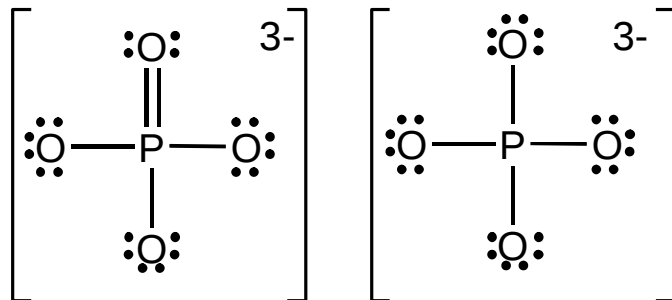
(a) Draw the other two resonance structures of N_2O .

(b) Provide formal charge calculations for these three resonance structures, and comment on the validity of the top resonance structure for its contribution to the properties of N_2O .

3. Two Lewis structures commonly used to represent the phosphate ion are shown below:

(a) Assign formal charges to all atoms in these dot structures

(b) Based on your work in (a), which of these two resonance structures is predicted to more accurately reflect phosphate ion?

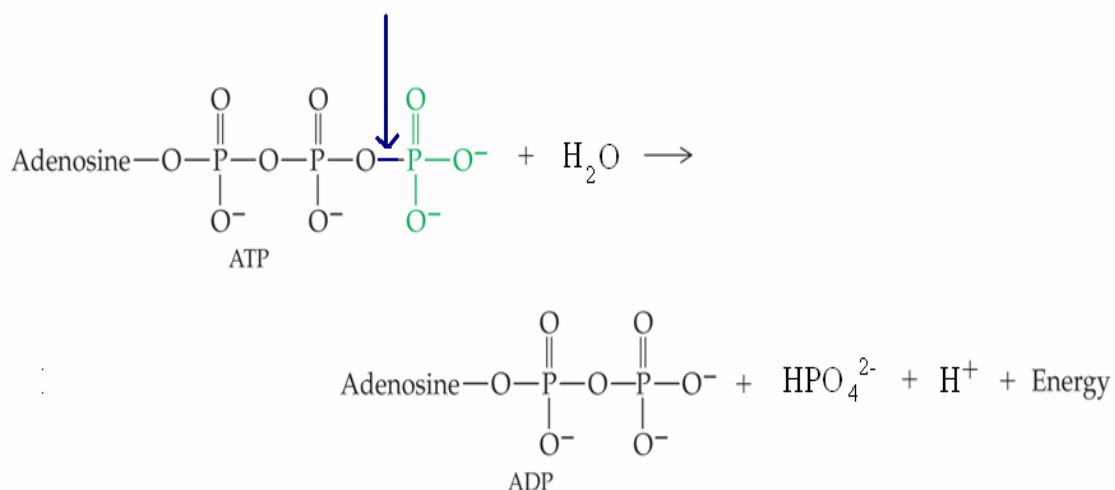


(c) Based on your answer to (b) are all phosphorus-oxygen bonds identical in this ion?

Geometry and Bonding: Post-Laboratory Questions

1. Amineborane (NH_3BH_3) is a compound attracting much interest because its high hydrogen content makes it a leading candidate for solid-phase hydrogen storage materials used in hydrogen-powered batteries.
 - (a) Sketch the Lewis dot structure for this molecule.
 - (b) Sodium borohydride (NaBH_4) and ammonium chloride react to form amineborane and two other common products, one is a gas and the other a solid. Provide Lewis dot structures for the ammonium and borohydride ions.
 - (c) Consider carefully the electrons represented in your dot structures above. Write the balanced equation for the reaction described in (b).
2. In each of the following cases, tell whether the bond angle increases, decreases, or is unchanged as a result of losing two electrons, converting the original anion into the cation shown.
 - (a) NO_2^- converted to NO_2^+
 - (b) ClF_2^- converted to ClF_2^+
 - (c) Defend one of your answers with clear dot and VSEPR sketches
3. The rapid interconversion of brown NO_2 to colorless N_2O_4 is an important reaction in the atmospheric nitrogen cycle. Review your dot structure drawn earlier for NO_2 . Sketch the plausible dot structure of N_2O_4 .

4. Hydrolysis of adenosine triphosphate (ATP^{4-}) to form adenosine diphosphate (ADP^{3-}) and a phosphoryl group is an extremely important reaction in biological systems. The conversion of ATP to ADP is responsible for the majority of energy used by the body to perform mechanical and chemical functions. This reaction is shown below.



- (a) Which of the phosphorus-oxygen bonds, the one broken in ATP (arrow) or the one formed in the new free phosphate/hydrogen phosphate ion, participates in resonance?
- (b) What effect does resonance have on the strength of the phosphorus-oxygen bond?
- (c) Which of the phosphorus-oxygen bonds is stronger, the one broken in ATP or the one formed in the new free phosphate/hydrogen phosphate ion? What effect does this have on the net energy change in this reaction?