

Chapter 4.1: Chemical Bonding

chemical bond →

→

ionic bond →



→

covalent bond →



Lewis structures →

→

→

<u>Element</u>	<u>Group</u>	<u># valence e⁻</u>	<u>Lewis Structure</u>
Li	1		
Be			
B			
C			
N			
O			
F			
Ne			

Lewis Structures of Ionic Compounds
Sodium and chlorine

Lewis Structures of Covalent Compounds
Hydrogen and chlorine

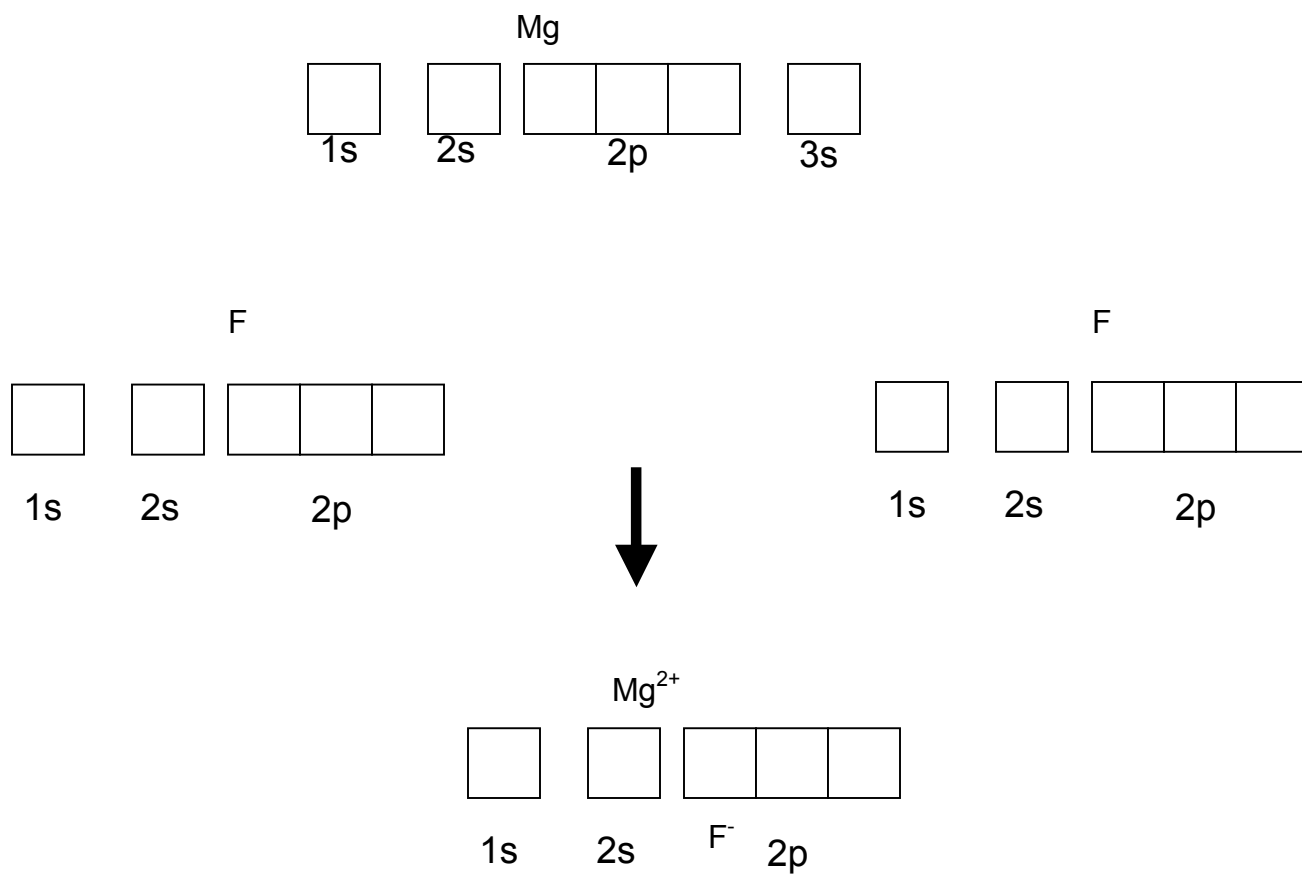
Example: magnesium reacting with fluorine

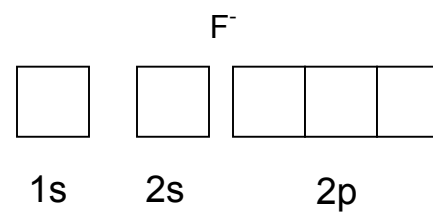
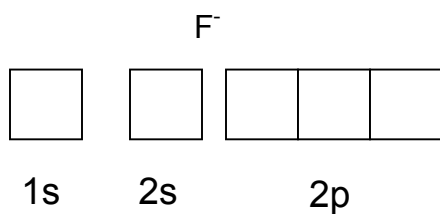


Lewis structures:

Electron configurations:

Orbital Box Diagram





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Covalent Bonding:

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Eg. Formation of F_2

Lone pairs of electrons are not involved in bonds

 F_2 – single bond – CO_2 – double bond – N_2 – triple bond –**Bond Energy:** energy required to break force of attraction between 2 atoms in a bond and separate them

∴

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Predicting Ionic and Covalent Bonds

Use differences in electronegativity between atoms

Electronegativity → a measure of an atom's ability to attract
electrons in a chemical bond

$\Delta E_n = 0 \therefore$ shared equally

$\Delta E_n > 1.7 \therefore$ ionic (transfer)

$\Delta E_n > 0.4 < 1.7$ polar covalent (unequal sharing) partial charges

$\Delta E_n = < 0.4$ – covalent no partial charges

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Metallic Bonding:

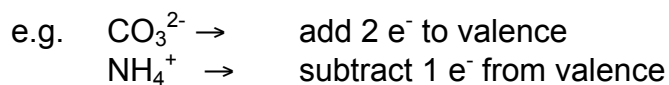
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Bond Type:

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- Called the “free-electron model” –
- Metallic bond is formed between the cations and the mobile electrons
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- Malleability and ductility –
-
- m.p. and b.p. – read independently and make notes

Drawing Lewis Structures for Polyatomic Ions and Molecules

1. Put the least electronegative atom at the center of the molecule; place other atoms around it with only single bonds.
2. Determine the total number of valence electrons in the molecule or ion (for polyatomic ions, pay close attention to charge).



3. Determine the total number of e^- needed for each atom to achieve a noble gas configuration.

4. Determine number of shared electrons: subtract 2) from 3) and divide by 2

5. Determine the number of non-bonding electrons: total valence e^- – shared e^-

Coordinate Covalent Bonds:

•
•

e.g. NH_4^+ total valence e^- Total e^- for noble gasNumber of shared e^-

 Number of lone pairs
 H_3O^+

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 $\text{O} - 1s^2, 2s^2, 2p^4$ **Resonance Structures:**

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i.e. SO_2

Experimental evidence suggests that the bonds are identical between the S and the O.

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Resonance structure shows the same relative position of the bond but has different places for bonding and lone pairs.

Resonance structures do not exist in reality i.e. the molecule is a hybrid of all the resonance structures.

Central Atoms with Expanded Valence Level

Possible to have more than 8 valence electrons in the central atom with some molecules and polyatomic ions.

Eg. PCl_5

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p.177#9-13 and p. 178 # 14-17

SCH 4U1 - TAKE HOME ASSIGNMENT

1. Draw the Lewis structure for the following polyatomic ions. Use the terms discussed in class to discuss the types of bonds in these molecules. What is special about b? Discuss.



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Laboratory Exercise:
Shapes of Molecules and Polyatomic Ions using the
Valence Shell Electron Pair Repulsion (VSEPR) Theory

Objectives

1. To relate the shapes and bond angles of chemical species to the number of electron pair domains in the valence shell of the central atom.
2. To relate molecular polarity to the shape and symmetry of the molecule.

Materials

A set of preassembled molecular models with the following shapes: linear, trigonal planar, tetrahedral, trigonal bipyramidal, octahedral, pentagonal bipyramidal (if available)

Introduction

One of the objectives of chemistry is to explain the properties of macroscopic samples in terms of the nature and behaviour of the molecules, atoms, or ions that make up the sample. For example, properties such as boiling point and water solubility depend on the extent of attraction between neighbouring particles in a sample. As you know from grade 11 chemistry, properties like boiling point and water solubility are influenced by the polarity of the individual molecules. That is, the characteristics of a polar substance will differ from those of a nonpolar substance. Polarity, in turn, depends on the three dimensional shape of the molecule and on the relative electronegativities of the atoms involved (recall Pauling's Electronegativity Scale and the Bonding Continuum).

Valence Shell Electron Pair Repulsion (VSEPR) Theory will allow you to predict the three dimensional shape of molecules and polyatomic ions. Once the three dimensional shape of a molecule is known, its polarity can be predicted.

The **Pauli Exclusion Principle** States that

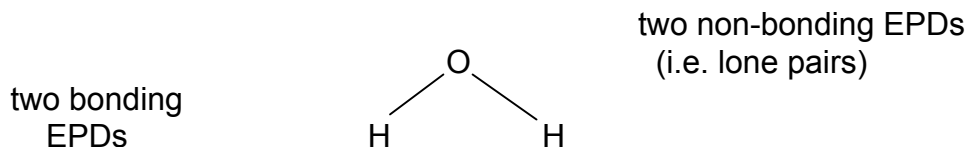
no two electrons within an atom can have the same set of four quantum numbers

or

no orbital can contain more than two electrons which must be of opposite spin.

We call a region in an atom where there is a high probability of finding two electrons of opposite spin an **electron pair domain (EPD)**. It is important to note that an electron pair domain can contain bonding electrons *or* non-bonding electrons (i.e. lone pairs).

Using a water molecule as an example, one can see four EPDs: two bonding EPDs and two non-bonding EPDs.



The Fundamental Principle of VSEPR Theory

A very simple yet extremely useful method of determining the geometry, or shape, of a molecule or polyatomic ion, is the **Valence Shell Electron Pair Repulsion** Theory. VSEPR Theory assumes that the EPDs(bonding and non-bonding) on an atom repel one another, and these repulsions determine the shapes of molecules and polyatomic ions.

That is, electron pair domains orient themselves around the *central atom* (O is the central atom in water for example) in a compound or in a polyatomic ion so as to minimize repulsion between them.

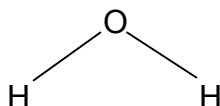
Each EPD, containing two electrons of opposite spin, tends to repel all other EPDs in the vicinity. To achieve a condition of minimum potential energy, it is necessary that the *electron pair domains be as far apart as possible*. In this position the electrostatic repulsion between the EPDs is at a minimum.

Around the central atom, we determine the "electronic geometry" by first counting the total number of EPDs in the valence shell of the central atom. The number of EPDs is determined by drawing the Lewis structure of the species in question. Remember the following:

1. VSEPR Theory is based on the premise that EPDs in a compound or polyatomic ion minimize repulsion by being as far apart from one another as possible. VSEPR Theory considers single, double and triple bonds each to be equivalent to one EPD. In other words, **VSEPR treats single, double, triple bonds the same.**
2. VSEPR theory considers lone pairs the same as bonding pairs: each is equal to one EPD. Think about it: Electron pair domains, whether they are bonding or non-bonding, repel other EPDs. All EPDs, bonding or non-bonding, have similar spatial requirements.

The main idea of VSEPR Theory is that electron-pair domains repel one another, so that they are arranged as far apart from one another as possible. The resulting arrangement of electron pair domains-bonded and non-bonded-is referred to as the **electronic geometry** of the central atom.

Important: Whenever there are lone pairs of electrons present, the actual, or **molecular geometry** will differ from the electronic geometry. Consider again the water molecule, H_2O , whose Lewis structure is



There are two bonding electron pair domains (i.e. the two O to H bonds); there are two lone pair electron domains on O for a total of 4 EPD. Hence, the **electronic geometry** (which considers only the total number of EPDs and NOT whether they are bonding or non-bonding) of water is tetrahedral. The actual, or **molecular geometry** (which takes into account any lone EPDs) of water is angular or bent, owing to the effect of the two non-bonding, yet space-demanding EPDs. Look at a molecular model of tetrahedral geometry, and of the water molecule to see this for yourself.

A good starting point for determining the electronic and molecular geometry of a given molecule or polyatomic ion is to draw the Lewis structure. Make sure that any lone electron pairs on the central atom are shown on the Lewis structure.

To recap: If any lone pairs are present, the electronic geometry will differ from the molecular geometry. Conversely, if no non-bonding EPDs are present, the electronic and molecular geometry will be the same.

We will examine various molecular models and build an understanding of the VSEPR Theory in a class discussion. As we go along, complete Table 1. You will need to draw the Lewis structure (assume all single bonds) and fill in the bond angles corresponding to each shape.