

CHEM 110: CHAPTER 8 Basic Concepts of Chem Bonding

Lewis Structures of Atoms: The Lewis Dot Diagram

Lewis Dot Diagrams (developed by chemist Gilbert Lewis) are used to indicate the number of valence e- for an atom and as a result are used in explaining chemical bonding in which one or more e- pairs are either shared (covalent bond) or transferred (ionic bond).

To draw a Lewis dot diagram, simply write the symbol for the element and use dots to represent electrons. The dots are placed at 12:00 and every 15 minutes thereafter clockwise. The dots should be left unpaired up to and including if 4 valence e- (e- = electron(s)) are present (the C family). Additional e- are paired up then.

THE NUMBER OF DOTS SHOULD EQUAL THE NUMBER OF VALENCE ELECTRONS IN THE ATOM.

The Ionic Bond

Recall that when a metal and non-metal combine chemically, an ionic bond usually results. This joining of atoms is due to a direct transfer of one or more electrons from one atom (usually a metal) to another atom (usually a non-metal). Positive (cations) and negative (anions) ions result and an ionic bond forms.

IN IONIC COMPOUNDS, CATIONS (formed by metals losing e-) ARE SMALLER THAN ANIONS (formed by non-metals gaining e-) AS THE

MORE NEGATIVE THE CHARGE, THE LARGER THE ION DUE TO INCREASING REPULSIONS (like charges repel and spread apart).

One can use the Lewis Dot Diagrams and knowledge of where the electron goes during a chemical reaction to explain how a given ionic substance forms.

Noble (Inert) Gas Electron Configurations and Predicting Formulae for Ionic Compounds

Atoms generally want to have a total of 8 valence e-. There is a special stability in acquiring this.

THE OCTET RULE: When atoms form chemical bonds they tend to want to acquire 8 valence e- (an octet). This is achieved by gaining (for non-metals) or losing (for metals) one or more e-.

Example 1

Using the e- configuration for F, how many e- would F need in order to have an octet of valence e-?

F has e- configuration: $1s^2 2s^2 2p^5 \rightarrow 7$ valence e-, so F needs one more e- from some other atom to give 8.

Example 2: Using the e- configuration for Na, how many e- would Na need to *LOSE* in order to have an octet?

Na has e- configuration: $1s^2 2s^2 2p^6 3s^1 \rightarrow 1$ valence e- so Na needs to lose 1 e- to have octet below 3s.

NOTE: Metals tend to lose e- while non-metals tend to gain e- in order to have an octet.

COVALENT BONDS

Recall that covalent bonds are usually between 2 metals or non-metals and are strong bonds formed by sharing e-.

Two e- being shared make up one covalent bond; this bond is termed a single bond.

Two pairs of e- being shared (4) make up a double bond; three pairs (6) make up a triple bond.

C-C is a single bond; C=C is a double bond; C≡C a triple bond between carbon atoms.

LINES INDICATE A PAIR OF ELECTRONS BEING SHARED.

If a bond results in *unequal* sharing of e-, it is termed a *polar covalent* bond. If equal sharing, a non-polar covalent bond results.

How do these bonds form? By orbitals (s, p, d, f) overlapping; the greater the overlap, the STRONGER the bond.

ELECTRONEGATIVITY

Electronegativity refers to the amount of attraction an atom has for its electrons. Metals tend to have low electronegativities (high electropositivities); while non-metals usually have high electronegativities (low electropositivities).

The electronegativity scale in use today was developed by Linus Pauling. The highest is 4.0 (F) and the lowest is 0.7 (Fr).

If the difference in electronegativity is zero or close to it, the bond is termed non-polar covalent.

Example: The C-C bond above would be non-polar covalent as the electronegativity difference is 0.

If the electronegativity difference is 0.5 or higher but less than 1.9, the bond is termed polar covalent. These bonds result in a DIPOLE forming.

A dipole results when 2 atoms of significant differing electronegativity share e- unequally. The result is a lop-sided e- cloud which indicates one atom controls most of the e-.

Finally, if the electronegativity difference is greater than 1.9, the bond is termed IONIC.

This indicates that electrons being shared by the atoms belong nearly entirely in control by one of the atoms (usually a non-metal) in the bond.

Example: When K bonds with Cl (electronegativity difference = $3.0 - 0.8 = 2.2$), the electron from K is transferred to Cl and Cl takes a negative charge (an anion, Cl^-); while K a positive charge (a cation, K^+). *See pg. 300 of text for further reading.*****

Lewis Structures for Compounds

Recall that the Lewis Dot Diagram simply indicates the number of e- with dots to represent valence (outermost, those involved in chemical bonding) electrons.

By combining Lewis Dot Diagrams for the elements in a compound, the LEWIS STRUCTURE can be obtained.

The following steps can be helpful in doing this.

- 1. Obtain the total number of valence e- by adding up the value for each of the atoms involved in the compound. If a negative ion is present, add an e-, if a positive ion, subtract an e- for +1, subtract 2 e- for +2, etc.*
- 2. Write the symbols for each of the atoms in the compound and connect them with a two dots or a single dash. NOTE: H*

atoms can form only one bond; O atoms do not usually bond to each other except in peroxides or superoxides. O can have a maximum of two covalent bonds. The halogens (F, Cl, Br, I) usually only form one bond.

- 3. Distribute pair(s) of e⁻ (dots) around each atom (EXCEPT H) to give each an octet (except H as it has only 2).*
- 4. If not enough e⁻ are around each atom, form double bonds by shifting a pair of e⁻ or if necessary triple bonds. Each bond counts for two e⁻.*
- 5. If the compound has a charge (an ion), put brackets [] around the structure and a superscript charge. []²⁻*

EXAMPLES: PF₃, H₂O, NH₄⁺, NO₃⁻

Resonance and Polyatomic Ion Containing Compounds Lewis Structures

Some compounds can have more than one Lewis structure. This is due to a bond (usually a double bond) shifting its location from the central atom to any of the other atoms attached to it.

All structures resulting from this are equivalent.

Ionic Bond Enthalpy

When an electron transfer occurs between 2 atoms (usually a metal with a non-metal), a large amount of energy is released (exothermic).

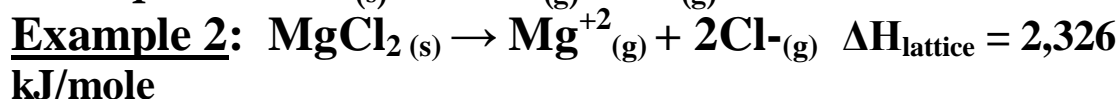
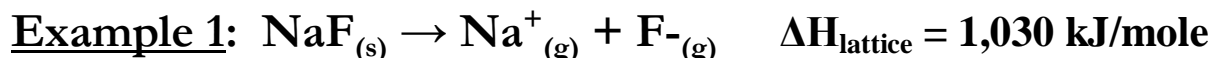
This release of energy is termed the ionic bond enthalpy (ΔH).



The reverse process would be endothermic:



Hence, it requires energy to separate an ionic compound into its ions. This quantity of E needed for separation of + and - ions into their gaseous phase is termed the *lattice E*.



AS CHARGE INCREASES, LATTICE ENERGY INCREASES.

See Table 8.2 pg. 293 for more values.

Calculating Lattice Energy

Lattice E cannot be determined directly by experiment; however, using Hess's Law of Enthalpy Summation and the Born-Haber Cycle it can be determined indirectly.

In this cycle, we consider the formation of an ionic compound from its elements by 2 different means:

- a. **Heat of Formation (ΔH_f): the direct path**
- b. **5 Steps involving :**
 - 1+ 2) **Formation of gaseous atoms of the ionic compound (endothermic)**
 - 3) **Removal of electrons from the metal (endothermic)**
 - 4) **and adding of those electrons to the non-metal (exothermic)**
 - 5) **Combining gaseous metal and non-metal ions to form an ionic compound ($-\Delta H_{\text{lattice}}$, exothermic)**

Dipole Moments

A dipole moment results when 2 electrical charges (of equal magnitude, but opposite sign) are separated by a distance.

Its value is termed a dipole moment, μ .

$\mu = Qr$, where Q = charge (Coulombs, usually 1.69×10^{-19} for an electron), r = distance (m)

A common unit for dipole moment is the DeBye (D).

$$1 \text{ DeBye} = 3.34 \times 10^{-30} \text{ C-m}$$

Example: Suppose the bond length is 2.07 Å, what would the dipole moment (μ) be?

$$\mu = 1.69 \times 10^{-19} \text{ C} \times 2.07 \times 10^{-10} \text{ m} = 3.312 \times 10^{-29} \text{ C-m}$$

Its value in DeByes would be,
 $3.312 \times 10^{-29} \text{ C-m} \div 3.34 \times 10^{-29} \text{ C-m/D} = 9.92 \text{ D}.$

Bond Enthalpies

The more E required to break a chemical bond between 2 atoms, the more stable (less likely to react/decompose) the bond is and hence the chemical compound.

The amount of energy (in kJ) required to break 1 mole of a particular bond in a gaseous compound is termed the bond enthalpy.

D (bond type) = bond enthalpy, ΔH always positive due to being endothermic

Example: D (C-I) = 240 kJ/mole, SEE TABLE 8.4 PG. 316 FOR MORE VALUES

The reverse process (forming bonds) would be exothermic.

Estimating Enthalpies of Reaction Using Bond Enthalpies

By knowing D (bond type) for each chemical bond represented in the reactants and products, one can calculate ΔH_{rxn} .

$$\Delta H_{\text{rxn}} = \Sigma \text{ broken bond enthalpies} - \Sigma \text{ formed bond enthalpies}$$



Bonds broken: 4 C-I + 2 Br-Br

Bonds formed: 4 C-Br + 2 I-I

$$\begin{aligned}\Delta H_{\text{rxn}} &= [4 D(\text{C-I}) + 2 D(\text{Br-Br})] - [4 D(\text{C-Br}) + 2 D(\text{I-I})] \\ &= [4 \cdot 240 + 2 \cdot 193] - [4 \cdot 276 + 2 \cdot 151] \text{ kJ} \\ &= 866 \text{ kJ} - 1406 \text{ kJ} = -540 \text{ kJ}\end{aligned}$$

Please note that this value is an estimate only.

As bond enthalpy \uparrow , bond length \downarrow .

As the number of bonds between 2 atoms \uparrow , bond enthalpy \uparrow
(stability \uparrow)

SEE TABLE 8.5 PG. 318 FOR AVERAGE BOND LENGTHS.