Molecular Structure and Bonding

Lecture 2

:

Lewis Theory

Lewis structures

The octet rule

All elements except hydrogen (hydrogen have a duet of electrons) have octet of electrons once they from ions and covalent compounds.

The Lewis dot symbols for atoms and ions shows how many electrons are need for a atom to fill the octet.

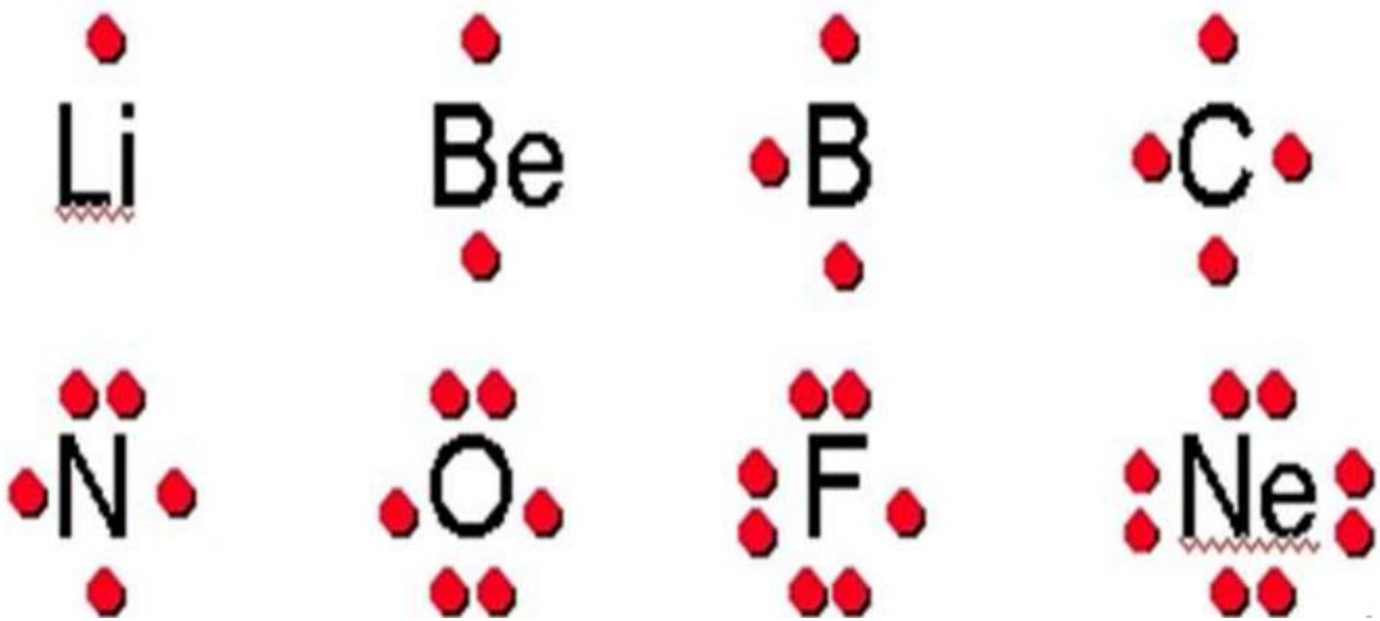
Normally there are octet of electrons on most monoatomic ions

Basic rules drawing Lewis dot symbols:

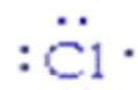
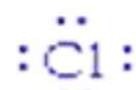
1. Draw the atomic symbol.
2. Treat each side as a box that can hold up to two electrons.
3. Count the electrons in the valence shell.

Start filling box – don’t make pairs unless you need to.

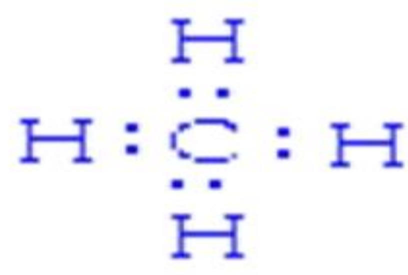
Lewis symbols of second period elements



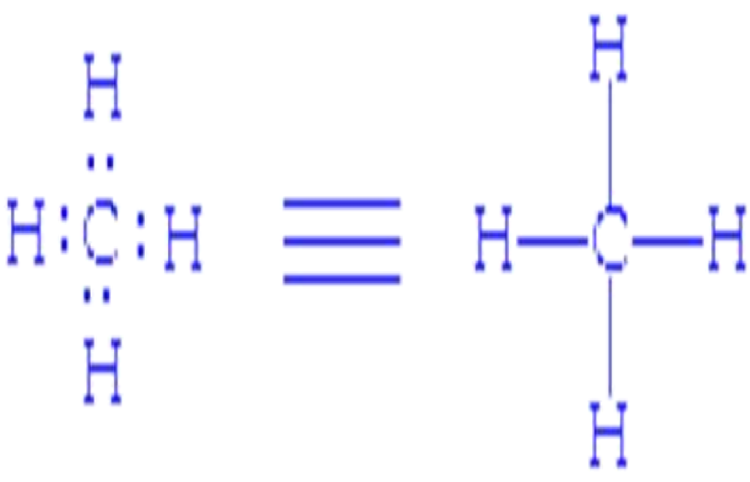
A Lewis symbol is a symbol in which the electrons in the valence shell of an atom or simple ion are represented by dots placed around the letter symbol of the element. Each dot represents one electron.

Hydrogen	$1s^1$	H·
Oxygen	$1s^2\ 2s^2\ 2p^4$	
Chlorine	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$	
Chloride ion	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$	

A covalent bond is a chemical bond formed by the sharing of a pair of electrons between two atoms. The Lewis structure of a covalent compound or polyatomic ion shows how the valence electrons are arranged among the atoms in the molecule to show the connectivity of the atoms

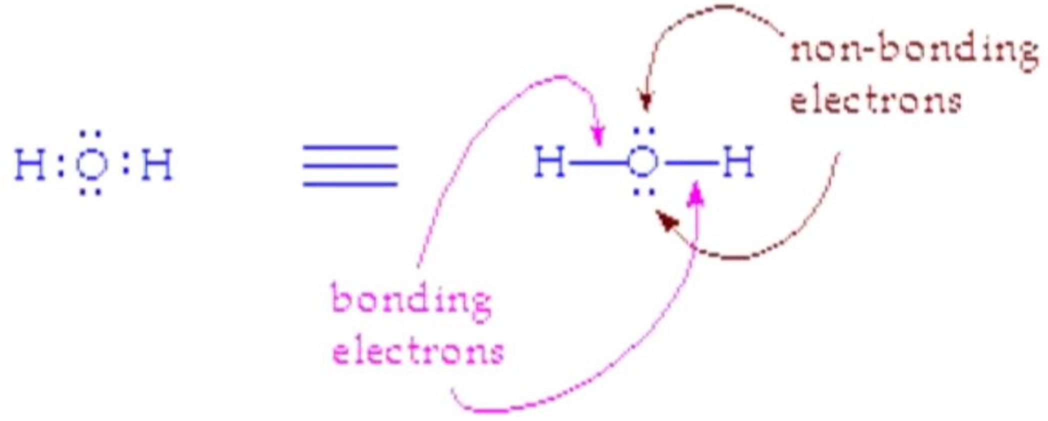


Instead of using two dots to indicate the two electrons that comprise the covalent bond, a line is substituted for the two dots that represent the two electrons.



The Lewis structure for water

Two hydrogens (H) are separately covalently bonded to the central oxygen (O) atom. The bonding electrons are indicated by the dashes between the oxygen (O) and each hydrogen (H) and the other two pairs of electrons that constitute oxygens octet, are called non-bonding electrons as they are not involved in a covalent bond.



Rules for getting Lewis Structures

1. Determine whether the compound is covalent or ionic. If covalent, treat the entire molecule. If ionic, treat each ion separately. For a monoatomic ion, the electronic configuration of the ion represents the correct Lewis structure. For compounds containing complex ions, you must learn to recognize the formulas of cations and anions.

2. Determine the total number of valence electrons available to the molecule or ion by:

(a) summing the valence electrons of all the atoms in the unit

(b) adding one electron for each net negative charge or subtracting one electron for each net positive charge. Then divide the total number of available electrons by 2 to obtain the number of electron pairs (E.P.) available.

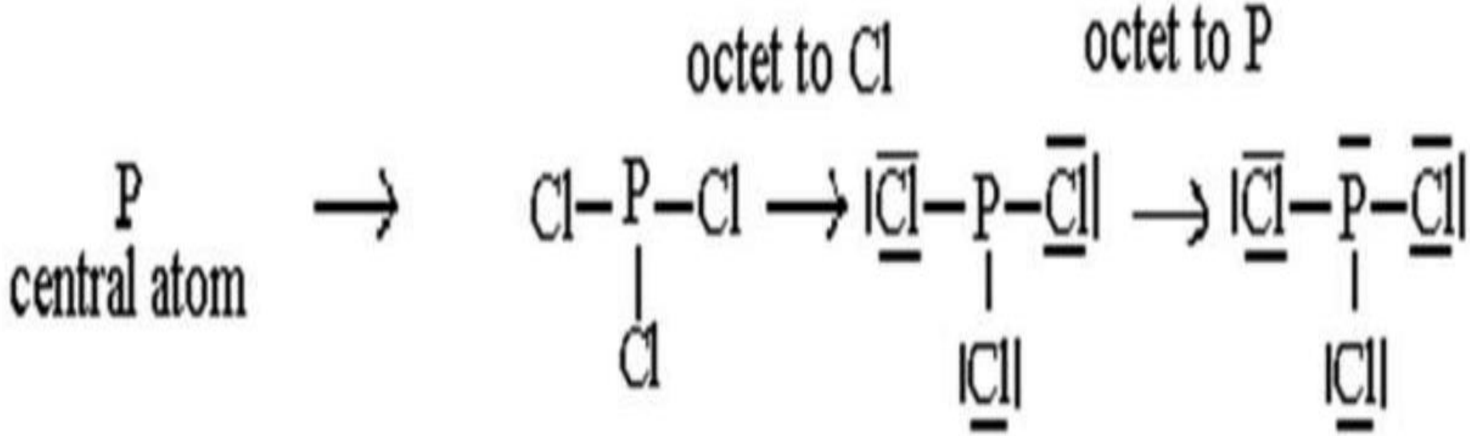
3. Organize the atoms so there is a central atom (usually the least electronegative) surrounded by ligand (outer) atoms. Hydrogen is never the central atom.

4. Determine a provisional electron distribution by arranging the electron pairs (E.P.) in the following manner until all available pairs have been distributed:

a) One pair between the central atom and each ligand atom.
b) Three more pairs on each outer atom (except hydrogen, which has no additional pairs), yielding 4 E.P. (i.e., an octet) around each ligand atom when the bonding pair is included in the count.
c) Remaining electron pairs (if any) on the central atom.

Lewis Structure of PCl_3 (atm.no. P=15, Cl=17)

1. Valence electrons: 5 + 3 x 7 = 26 (13 pairs)
2. Central atom is P
3. Connect the terminal atoms to central atom
4. Give octet to P and give octets to Cl
5. Count electron pairs: 3 bond pairs = 3 pairs 1 + 3 x 3 = 10 lone pairs = 10 pairs



13 pairs

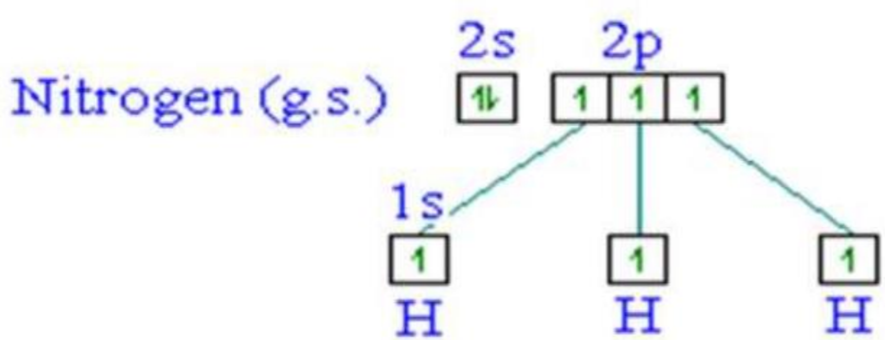
Types of Electrons Pairs

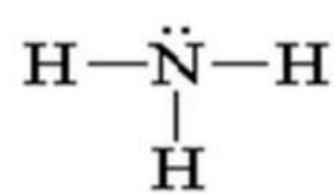
Bond pair: electron pair shared between two atoms.

Lone pair: electron pair found on a single atom. Molecules obeying the octet rule.

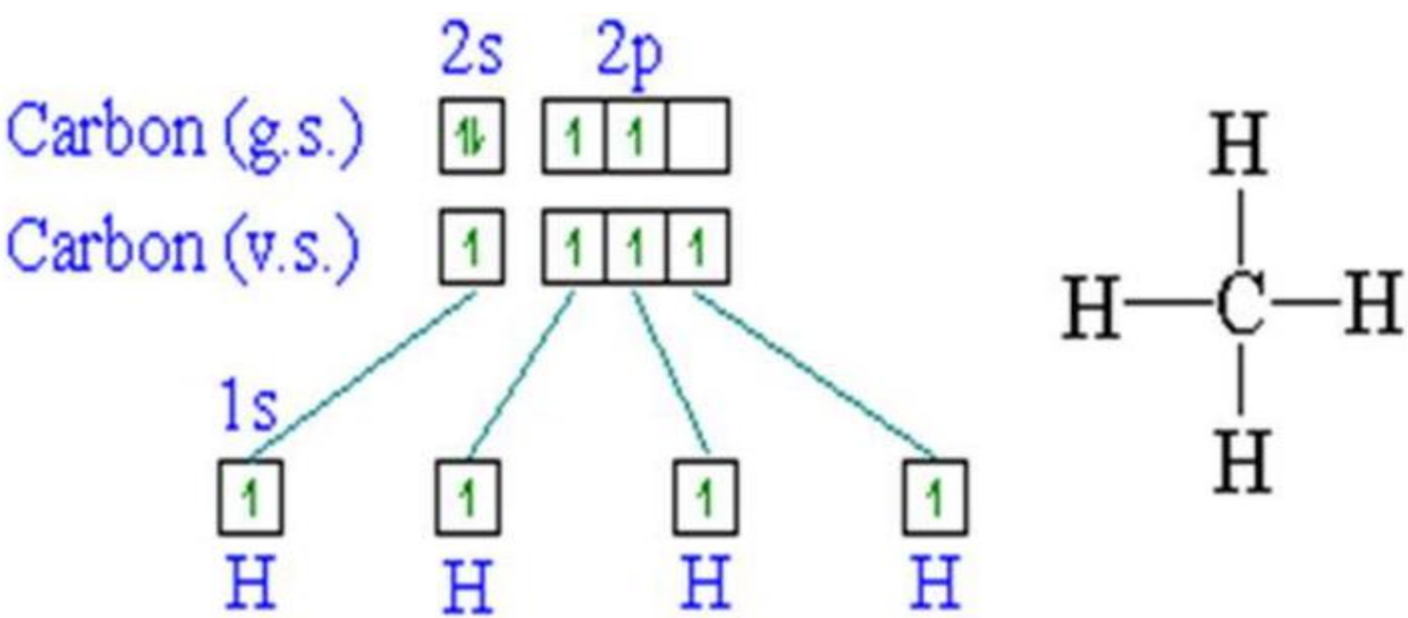
In many molecules, each atom **(except hydrogen)** is surrounded by eight bonding or lone-pair electrons. There is a special stability associated with this configuration. Examples are water, ammonia and methane.

The ground state (g.s.) configuration of N has three unpaired electrons. Each hydrogen atom has one. No rearrangement is necessary to make the three N–H bonds. Be sure to mark the lone pair on the Lewis diagram.





The ground state of carbon has only two unpaired electrons, but it is necessary to make four bonds to the hydrogens. The solution, in this case, is to promote a 2s electron to the empty p orbital. Then four bonds can be made. SiH4 has the same Lewis Structure as CH4



Molecules with multiple bonds:

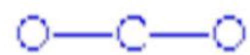
Examples: Consider carbon dioxide CO2

1-The first step in drawing Lewis structures is to determine the number of electrons to be used to connect the atoms. This is done by simply adding up the number of valence electrons of the atoms in the molecule

carbon (C) has four valence electrons x 1 carbon = 4 e^-
oxygen (O) has six valence electrons x 2 oxygens = 12 e^-

There are a total of 16 e - to be placed in the Lewis structure

1. Connect the central atom to the other atoms in the molecule with single bonds.
   Carbon is the central atom, the two oxygens are bound to it and electrons are added to fulfill the octets of the outer atoms.

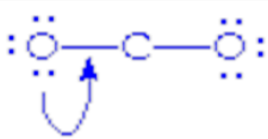
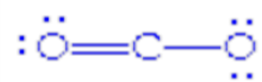
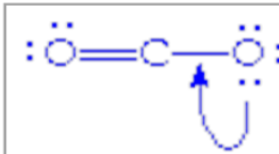


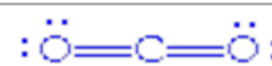
2. Complete the valence shell of the outer atoms in the molecule.

3. Place any remaining electrons on the central atom.

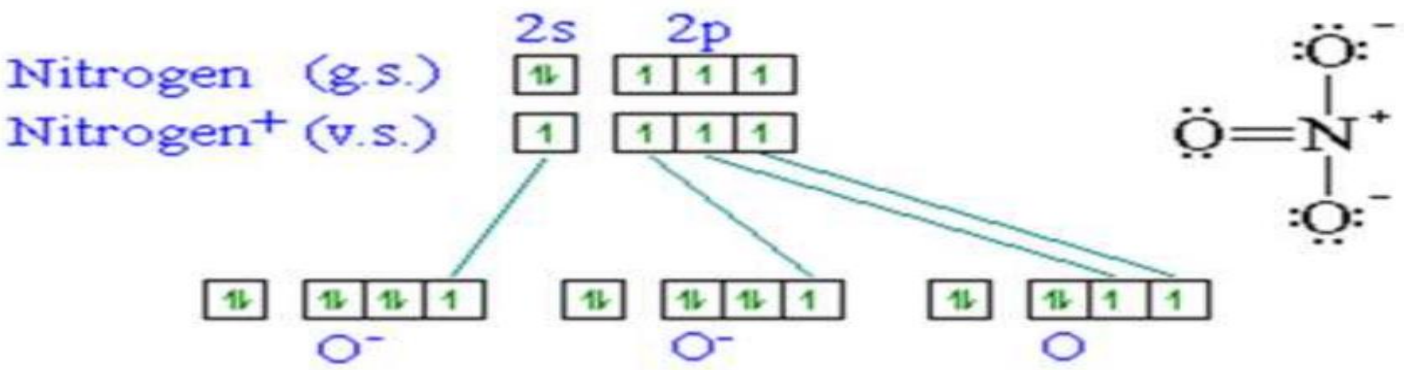
There are no more electrons available in this example.

1. If the valence shell of the central atom is complete, you have drawn an acceptable Lewis structure.
   Carbon is electron deficient - it only has four electrons around it. This is not an acceptable Lewis structure.
2. If the valence shell of the central atom is not complete, use a lone pair on one of the outer atoms to form a double bond between that outer atom and the central atom. Continue this process of making multiple bonds between the outer atoms and the central atom until the valence shell of the central atom is complete.

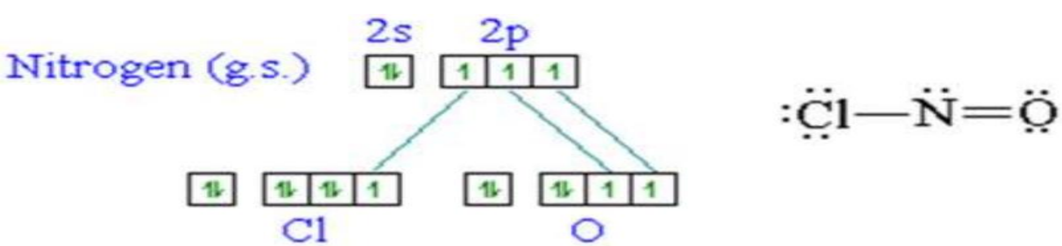
	Becomes	
The central atom is still electron deficient, so share another pair.		

The best Lewis structure that can be drawn for carbon dioxide is:. 

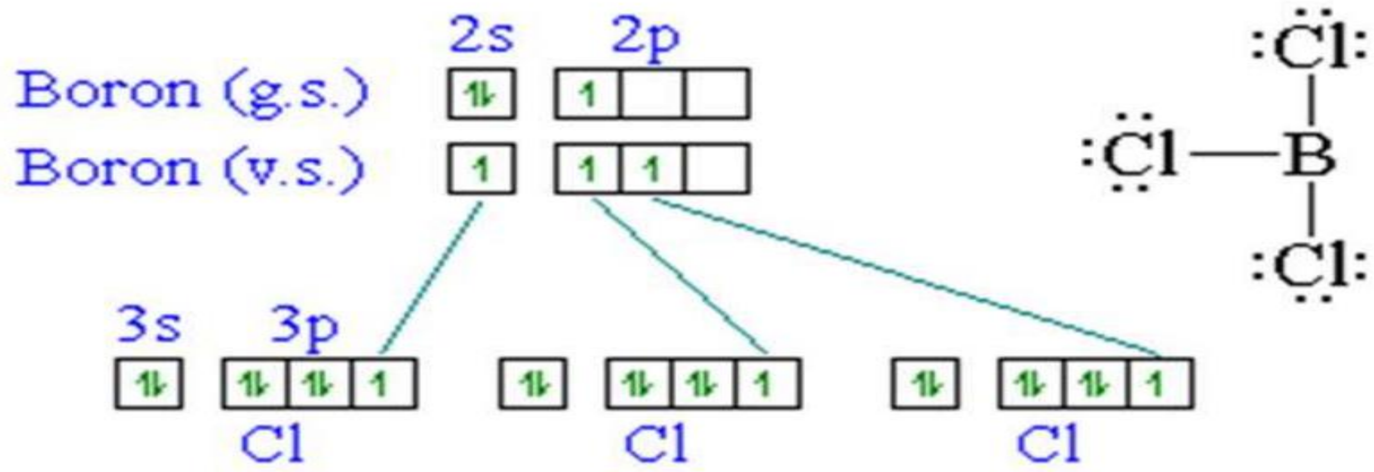
Lewis Structure of nitrate anion and nitrosyl chloride NOCl



Neutral nitrogen has 3 unpaired electrons You must move one electron from nitrogen to a neutral oxygen to get the configurations shown.



Lewis Structure of BCl3



The boron must be in a suitable valence state to bind to the three chlorines.

Lewis Structure of PCl_5

i) Count the total valence lectrons: $5 + 5 \times 7 = 40$ (20 pairs)
ii) P is central atom:
iii) P already have 5 electron pairs then give octets to Cls
iv) count electron pairs.

5 pairs on P = 5
5 x 3 pairs on Cl = <u>15</u>
20 electron pairs