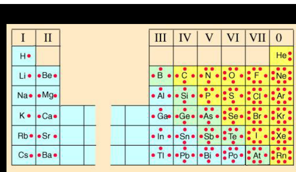
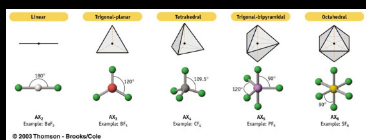


Lewis Dot Formulas



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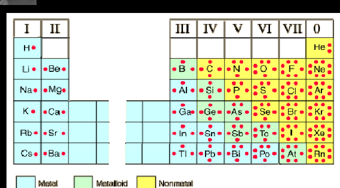
Lewis Dot Formulas

Gilbert Lewis (1916)
Valence electrons represented by dots around a core
Elements have "A" group number of valence electrons

Tool for explaining bonding between atoms



Members of a Chemical Family have same Lewis Dots

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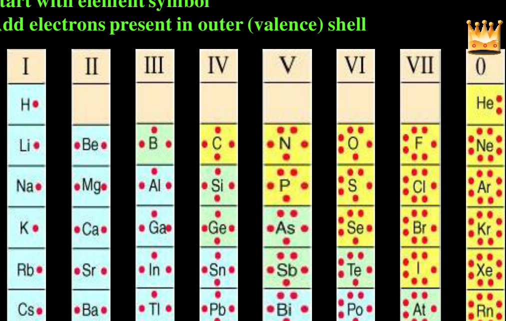
Lewis Dot Formula - Atoms

Start with element symbol
Add electrons present in outer (valence) shell



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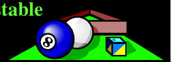
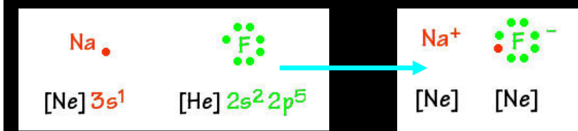
Octet Rule

Eight valence electrons, ns^2np^6, is especially stable
Noble gases do not tend to form compounds



To reach stability of the octet:
Atoms lose or gain (transfer) electrons (for ionic compounds)
Atoms share electrons (for molecular or covalent bonded compounds)



Product: both atoms with "inert configuration"

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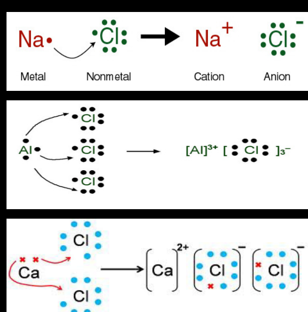
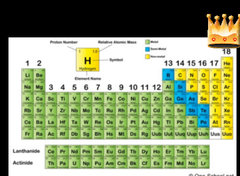
Lewis Dot Formula – Ionic Compounds

Electrons transferred from metal to non-metal





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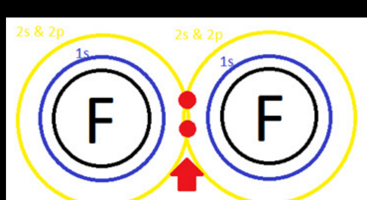
Covalent Bond: Electrons Shared



Electron pair BETWEEN atoms implies sharing
Both atoms "noble"
Each shared pair = covalent bond

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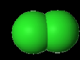
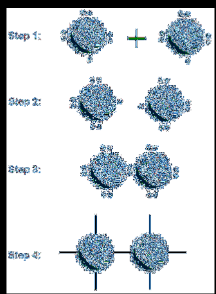
Nomenclature – Line for pair
Example: Diatomic Halogen





Draw Valence Electrons

Establish "share" or "transfer"

Connect "Share"

Can replace any 2 e^- with line

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Lewis Dot Formula - Compounds

molecule	Lewis structure	# regions of high electron density	molecule	Lewis structure	# regions of high electron density
$BeCl_2$	:Cl–Be–Cl:	2	BF_3	:F: / B / :F: :F:	3
HCN	H—C≡N:	2	SO_3	:O: ‖ S / :O: :O:	3
CO_2	O=C=O	2	NO_2	O=N–O:	3
CH_4	H / C–H / H H	4	NH_3	H / N / H H	4
PCl_5	:Cl: / :Cl–P–Cl: / :Cl: :Cl:	5	SF_6	:F: / :F: S :F: / :F: :F: / :F:	6

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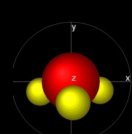
Lewis Dot Formulas

Useful for simple ions
Rapidly becomes tedious
Typically, does Not provide stereochemistry

H : N : H
H

Ammonia



Chemistry is a 3-D Phenomenon
2-D thinking limits horizons & understanding

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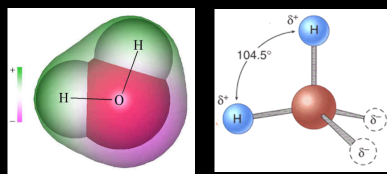
Valence Shell Electron-Pair Repulsion
VSEPR (“Ves-per”)

Unshared Pairs Repel – maximize distance between pairs
Creates Molecular Geometry



Extension of Lewis Dot Structures

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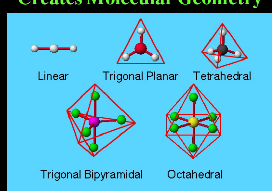
Valence Shell Electron-Pair Repulsion
VSEPR (“Ves-per”)

Unshared Pairs Repel – maximize distance between pairs
Creates Molecular Geometry



Extension of Lewis Dot Structures

Beyond CEM 101 Level

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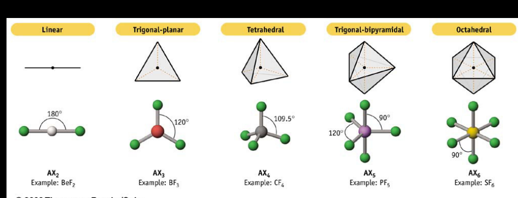
Valence Shell Electron Pair Repulsion (VSEPR)

Central Atom Bonding Determines Molecular Shape

Number of electron bonding groups:

2 3 4 5 6



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VSEPR: Lone Pair Repulsion Finalizes Shape

Groups

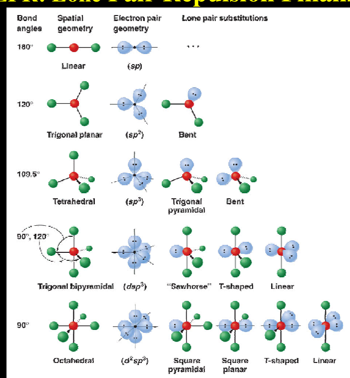
2

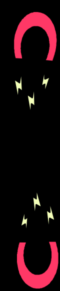
3

4

5

6





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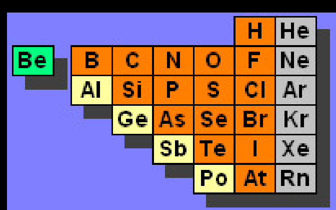
Valence Shell Electron-Pair Repulsion

Uses unshared electrons to predict molecular shape



Primarily used with non-metal central atoms

('cause they have more electrons)

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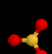

Drawing Lewis Structures

SO_3

Major pollutant in power plant emissions

$SO_3 + H_2O \rightarrow H_2SO_4$

Electronegativity:

S = 2.5

O = 3.5

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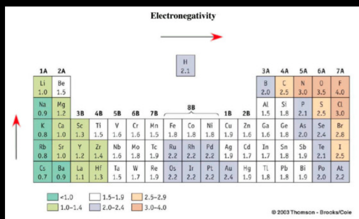
Step One: Determine Least Electronegative Atom



Least Polar Atom
Becomes Central
In Lewis Structure

H never Central

Electronegativity Differences

Δ ≤ 0.4 ➔ non-polar covalent
Δ > 0.4 - 1.9 ➔ polar covalent
Δ> 1.9 ➔ ionic

Δ = difference in electronegativity of the bonded atoms

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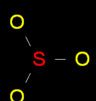
Step Two: Calculate Valence Electrons for Each Atom



Sum the valence electrons of all the atoms in the unit
Add one electron for each net negative charge
Subtract one electron for each net positive charge

For SO_3:
S = 6 electrons
O = (3 x 6) = 18 electrons
Total = 24 electrons

Divide by 2 to get number of electron pairs
24 electrons / 2 = 12 electron pairs

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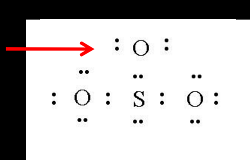
Step Three: Distribute Electrons around Central Atom

One pair between the central atom and each ligand atom
Central atom filled to octet
Additional pairs on each outer atom (except hydrogen)

For SO_3 ➔ Drawing to total of 12 pairs

Not Octet



Not all atoms have octet

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Step Four: Use "Formal Charge" to Resolve Octets

Need Formal Charge to be 0 on all atoms
or the charge on ionic species

Formal Charge = # valence e^- – (# unshared e^- + 0.5 * bonding e^-)

For Sulfur (the central atom)

F = 6 (group 6 atom) – (2 +3 (6/2))

F = 6 – 5 = +1

In terms of "molecular Psychology"
Sulfur not "happy" with a full +1 charge

Reduce formal charge with multiple bond formation

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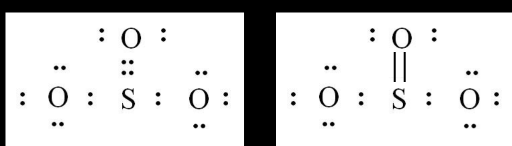
Step Five: Add multiple bond to complete octet



Step Six: Recalculate Formal Charges

Sulfur: 6 – (0 +4) = +2
Oxygen in bottom row: 6 – (6 + 1) = -1
Oxygen at top: 6 – (4+2) =0
Formal Charges balance: 2 x (-1) electrically balances +2

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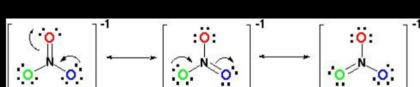
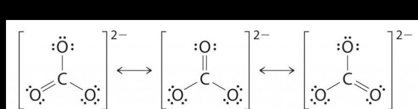
Resonance

Concept used to explain observed bond lengths

Describes molecules where bonding cannot be expressed with a single Lewis Structure
Electrons assumed to be delocalized throughout the system
Result is defined as a "resonance hybrid" of several forms
Individual resonance structures do not exist





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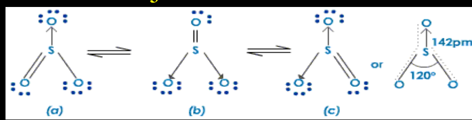
SO_3: Resonance Stabilized



STRUCTURAL CALCULATIONS

Molecular Formula: SO_3
Systematic Name: Sulfur Trioxide

Central Atom: S (Sulfur)

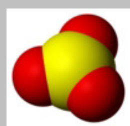
Valence Electrons: 24
Total Electrons: 40

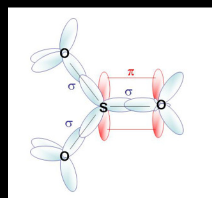
Bonded Pairs: 3
Lone Pairs: 0
Electron Pairs: 3

Single Bonds: 2
Double Bonds: 1
Triple Bonds: 0

XAX Bond Angle: 120°

EP Arrangement: Trigonal Planar
Molecular Geometry: Trigonal Planar
VSEPR Notation: AX_3





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Bond Order

Covalent Bonds: Number of electron pairs in the bond

$C \equiv C$ $C = C$ $C - C$

Bond Order: 3 2 1

Resonance Bonds: # Electron Pairs / Total Bonds of same type

$O = N - O \longleftrightarrow O - N = O$

$$\text{Bond Order} = \frac{3\ e^-\ \text{Resonance Pairs}}{2\ N\text{—}O\ \text{Bonds}} = 1.5$$

> Bond Order: Shorter and stronger the bonding between atoms

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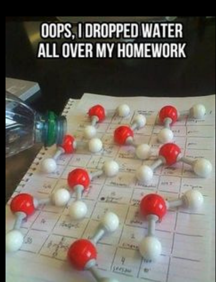

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