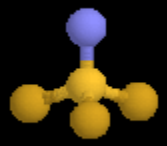
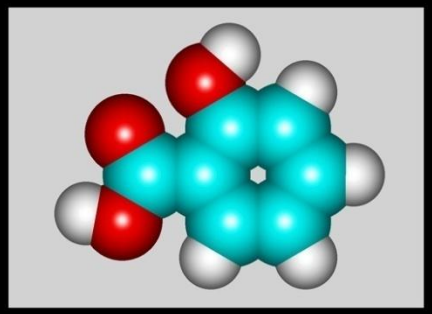
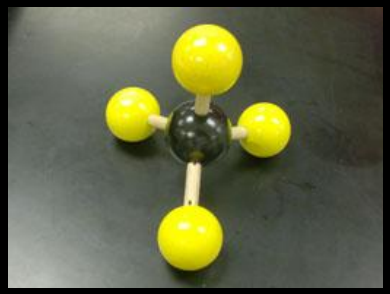
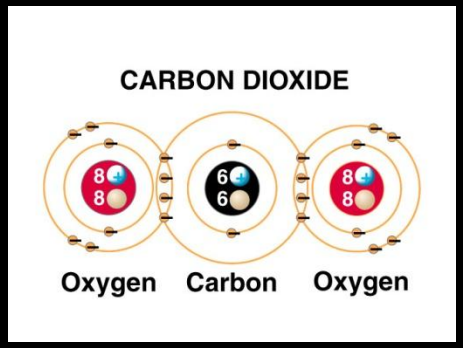
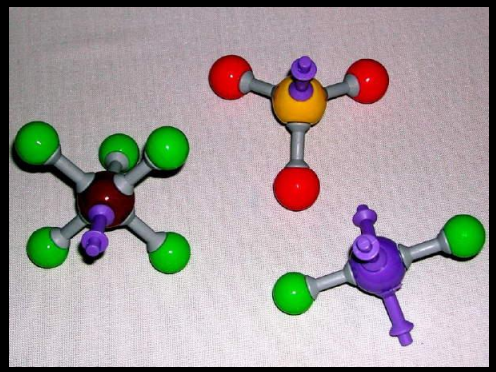


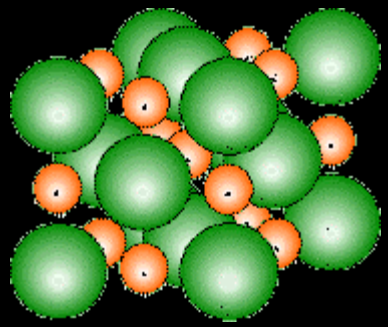




Chemical Bonds & Modeling







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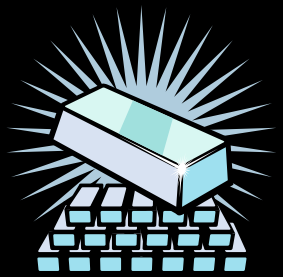
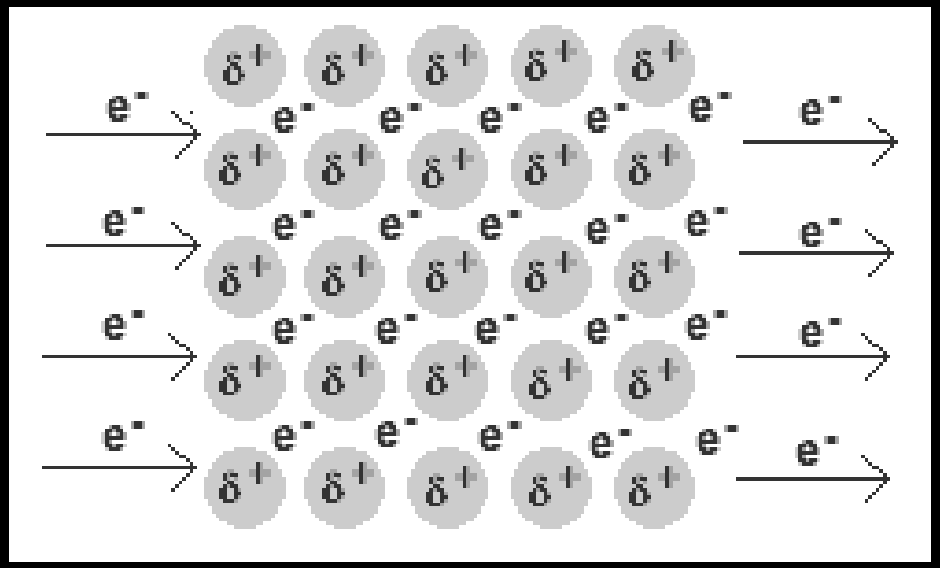
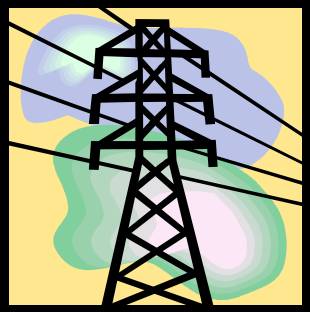
Metallic Bonding



“Sea of Electrons” floating in metal cation matrix
Electrons not attached to any specific cation





Explains current flow

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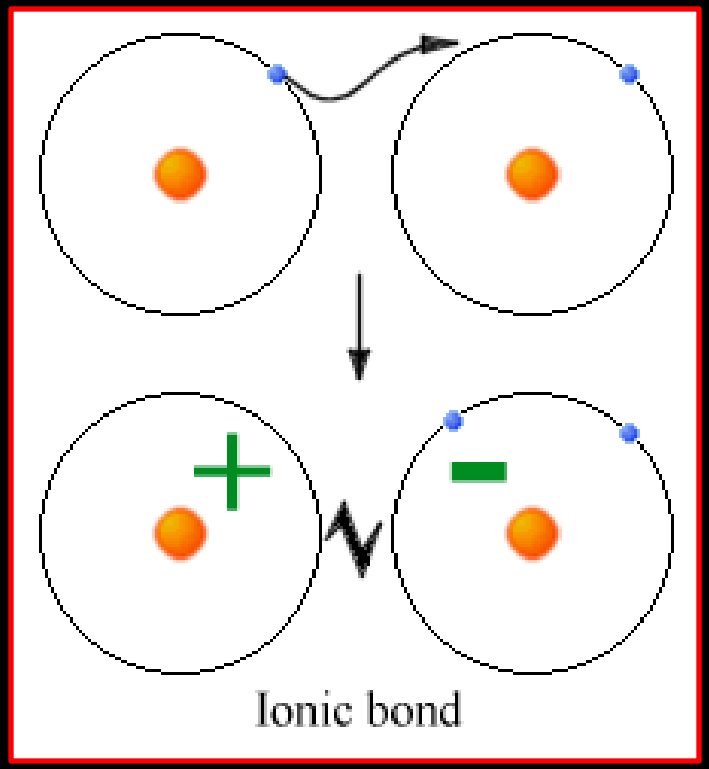
Ionic Interactions

Total Transfer of electrons
Result = cation & anion
Held together by electronic interactions



Ionic bond

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Ionic Interactions

+1	+2												-3	-2	-1	
+1	+2										+3		-3	-2	-1	
+1	+2	+3	+2 +3 +4	+2 +3 +5	+2 +3 +4 +6	+2 +3 +4 +7	+2 +3	+2 +3	+1 +2	+1 +2	+2	+3	+4	-3	-2	-1	
+1	+2	+3	+4	+3 +5	+3 +6	+4 +6 +7	+3 +4	+3	+2 +4	+1	+2	+3	+4	+5	-2	-1	
+1	+2	+3	+4	+5	+6	+4 +6 +7	+3 +4	+3 +4	+2 +4	+1 +3	+1 +2	+3	+4	+5	+6	-1	
+1	+2	+3	+4									+3	+4	+5	+6		

+3 +4	+3	+3	+3	+2 +3	+2 +3	+3	+3	+3	+3	+3	+3	+2 +3	+3
+4	+4 +5	+3 +4 +5 +6	+3 +4 +5 +6	+3 +4 +5 +6	+3 +4 +5 +6	+3 +4	+3 +4	+3 +4	+3	+3	+2 +3	+2 +3	+3

Atoms gain/lose electrons to mutually become "Noble"

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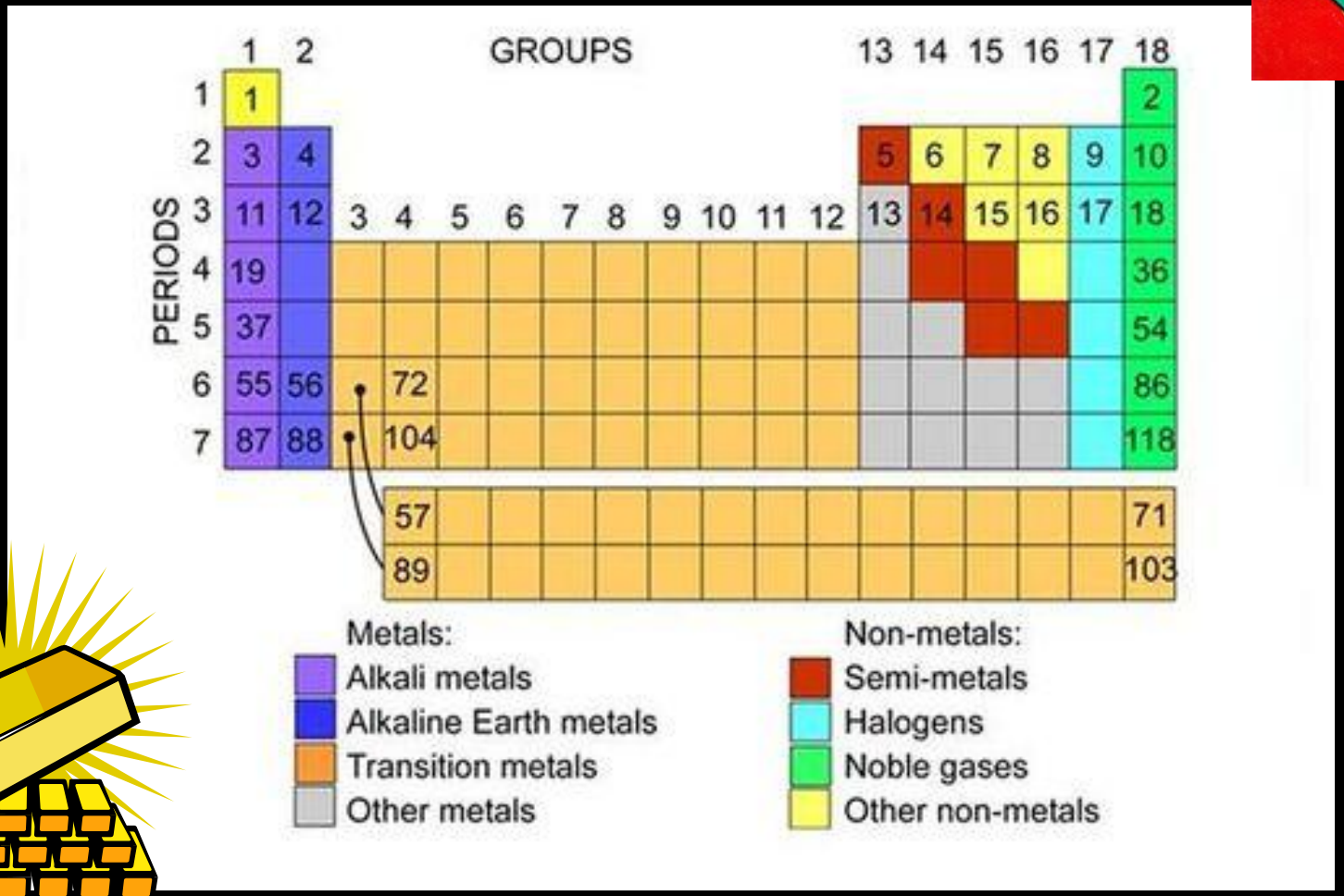
Gain or Lose Electrons?

Metals ➔ lose electrons
Non-Metals ➔ gain or share



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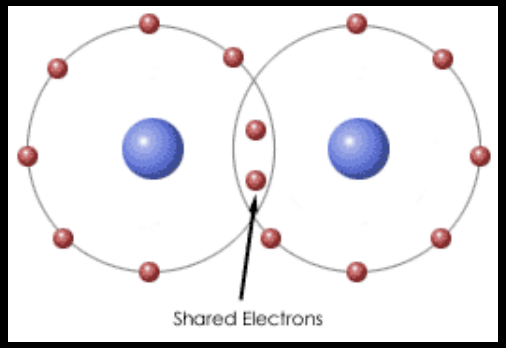
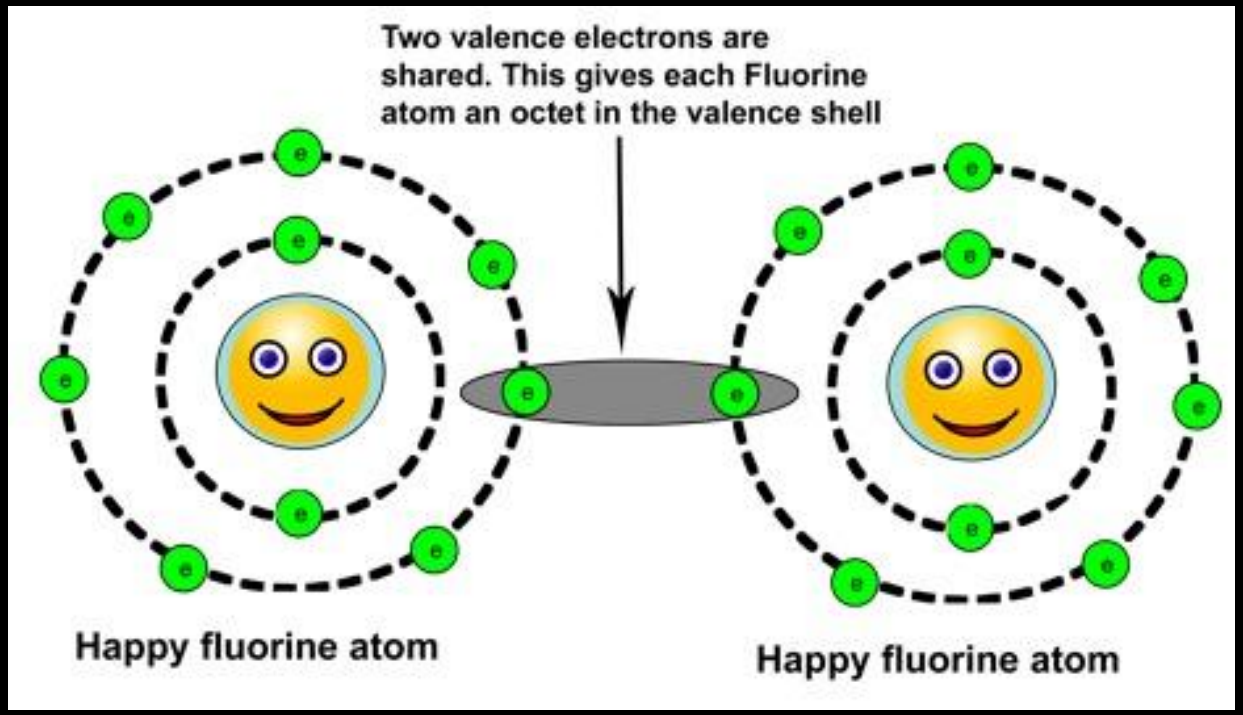
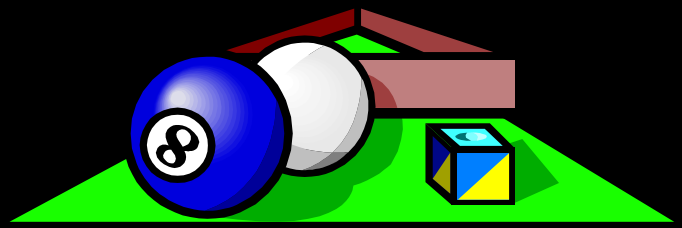
Covalent Bonding

Atoms share electrons to complete "Octet"







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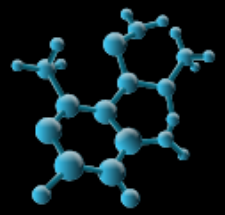
Electronegativity Differences

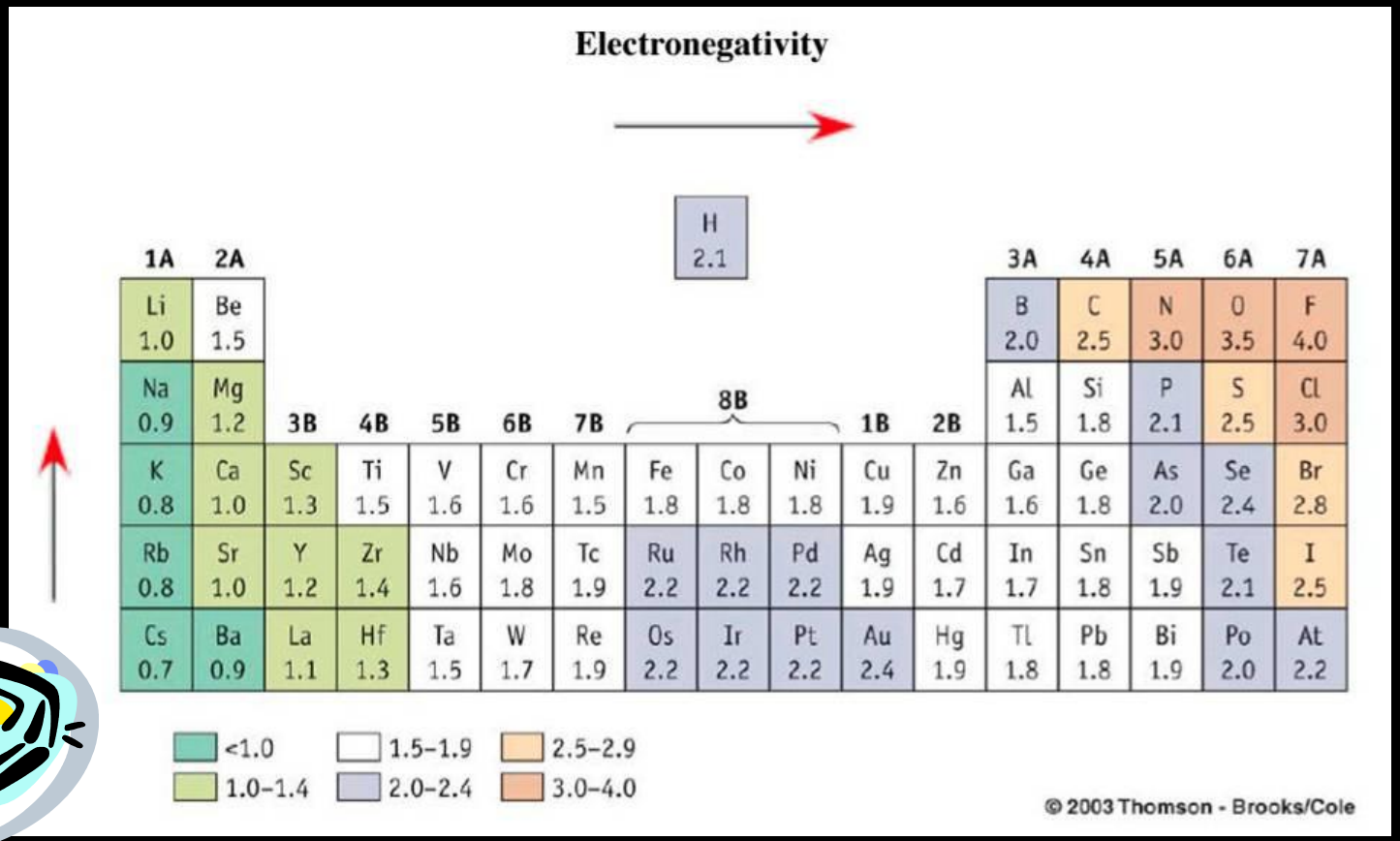


$\Delta \leq 0.4$ ➔ non-polar covalent

$\Delta > 0.4 - 1.9$ ➔ polar covalent

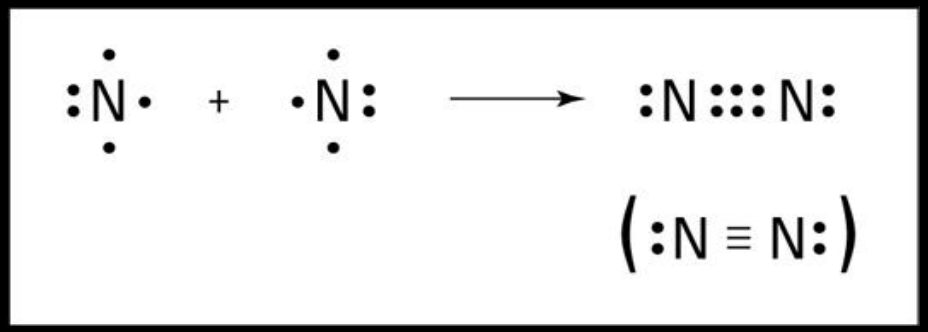
$\Delta > 1.9$ ➔ ionic

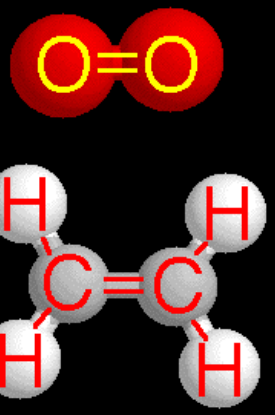
Δ = difference in electronegativity of the bonded atoms



Multiple Bonding

Atoms reach octet by sharing more than one pair of electrons
Each shared pair constitutes a bond
One shared pair = single bond
Two shared pairs = double bond
Three shared pairs = triple bond





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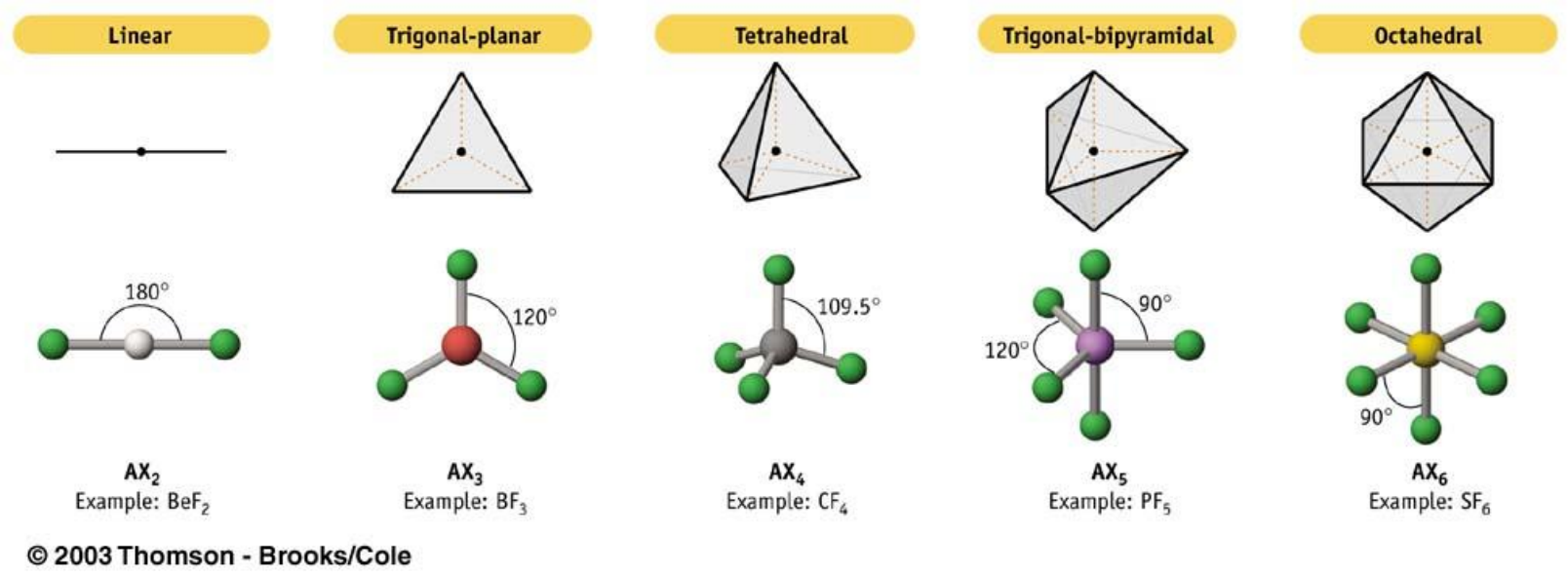
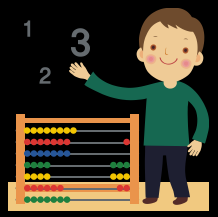
Central Atom Bonding Determines Molecular Shape

Number of electron bonding groups:

2 3 4 5 6





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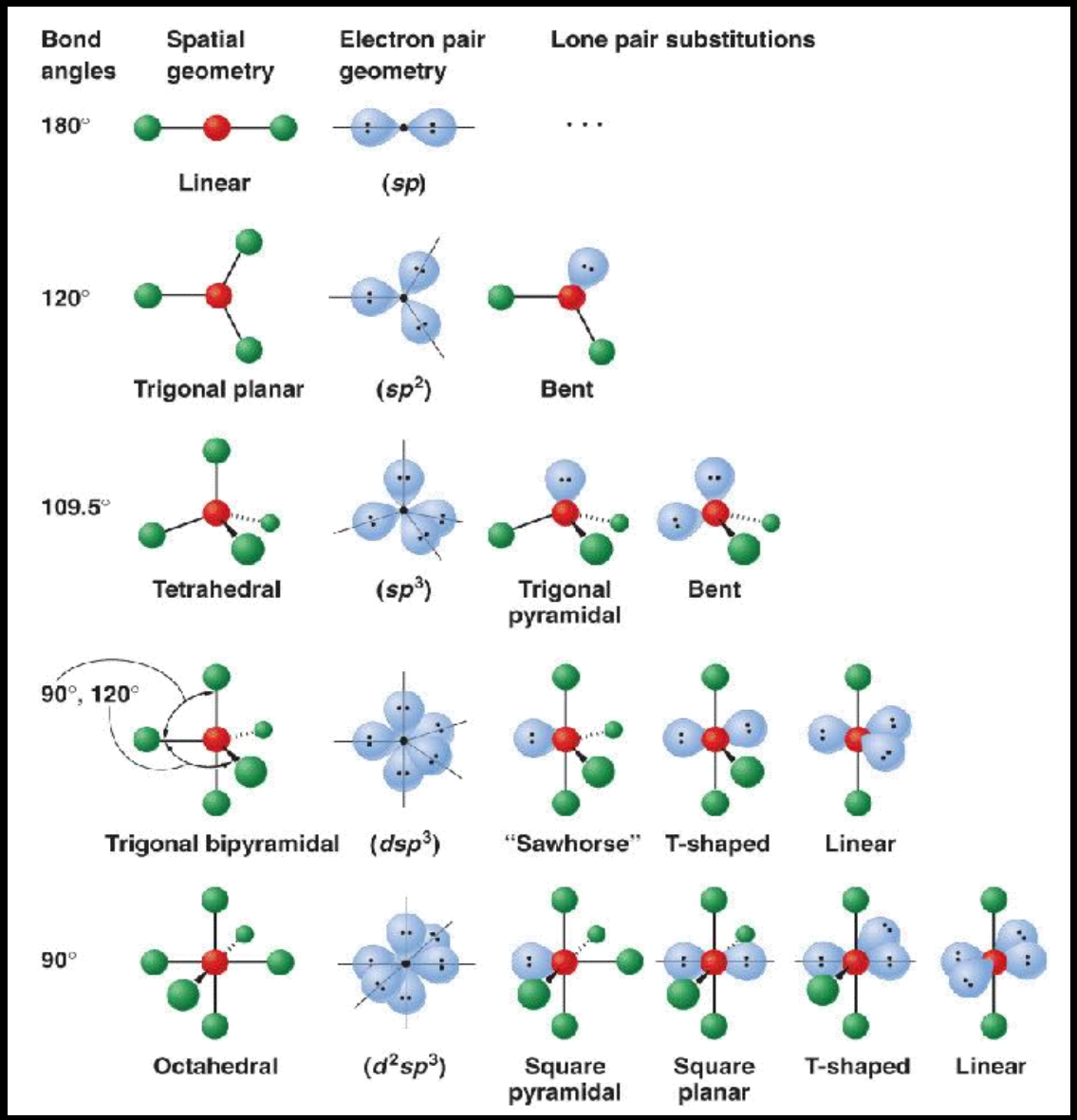
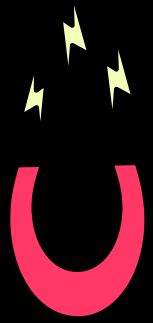
Lone Pair Repulsion Finalizes Shape

# Groups	Bond angles	Spatial geometry	Electron pair geometry	Lone pair substitutions
2	180°	Linear	(*sp*)	. . .
3	120°	Trigonal planar	(sp^2)	Bent
4	109.5°	Tetrahedral	(sp^3)	Trigonal pyramidal; Bent
5	90°, 120°	Trigonal bipyramidal	(dsp^3)	"Sawhorse"; T-shaped; Linear
6	90°	Octahedral	(d^2sp^3)	Square pyramidal; Square planar; T-shaped; Linear



Maximize distance Between electron pairs



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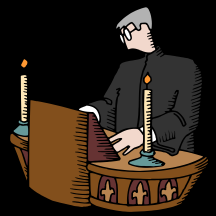
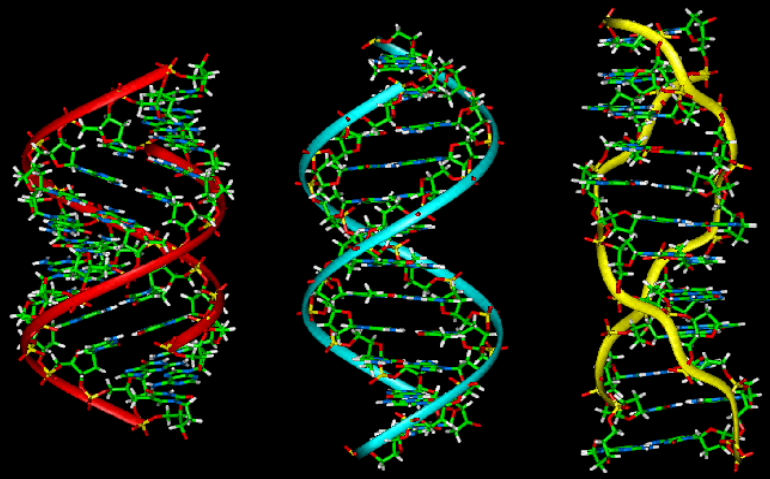
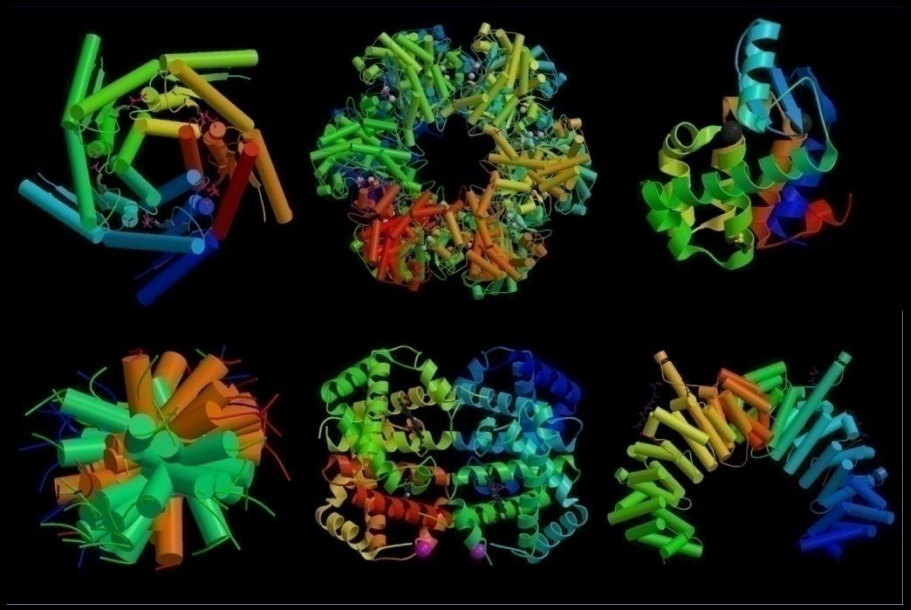
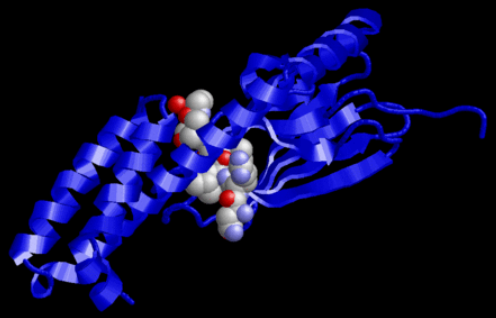
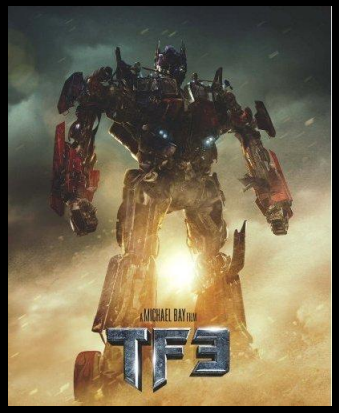
Basic Chemical Theology; Form & Function Intimately Related











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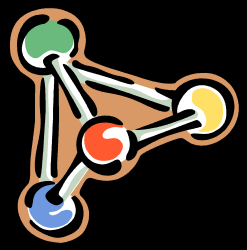
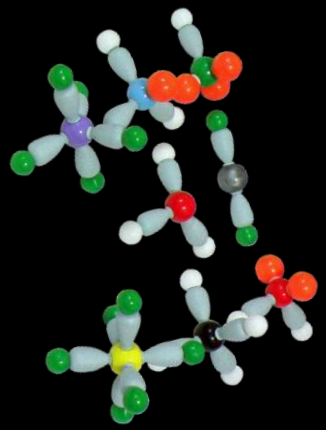


Modeling Lab



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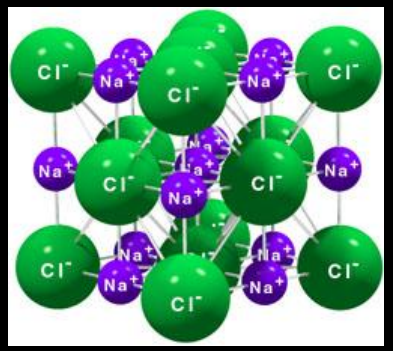
Today's Lab

Purpose

To observe models of ionic and covalent compounds
To build models of covalent compounds

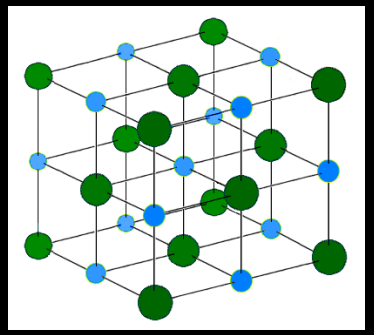


Chemical Bonding Video

Model of an Ionic Crystal

Create a data table

Observe the model of the sodium chloride (NaCl) crystal
Describe its shape (Cubic)
Are there any independent units that are "molecules" of NaCl? (No)
What is the ratio of number of Na^+ to Cl^- ions? (1:1)



Making Models (Work in pairs)

Examine each of the different spheres.

Count & record the # holes (# bonds) in each

Element	Symbol	Color	# bonds	Element	Symbol	Color	# bonds
Hydrogen	H	white	1	Nitrogen	N	Blue	3 (4)
Chlorine	Cl	green	1	Oxygen	O	Red	2 (4)
Carbon	C	black	4				

Rules for constructing molecular models:

- The color code tells you which sphere to use.
- The subscripts tell you how many of the atoms to use.
- All bonds (holes) must be used.
- All bonds must connect to atoms at both ends.
- Use short sticks for single bonds (one shared pair of electrons).
- Use longer, flexible sticks for multiple bonds.

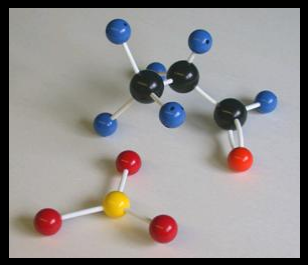
Construct each of the following models

The gases in air:

- oxygen, O_2
- nitrogen, N_2

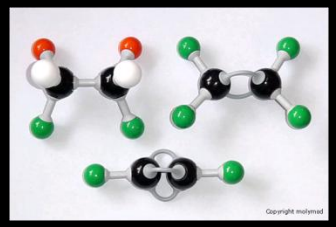
The "greenhouse gases"

- carbon dioxide, CO_2
- methane, CH_4



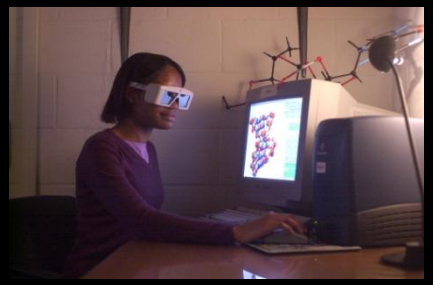
Others:

- water, H_2O
- ammonia, NH_3
- carbon tetrachloride, CCl_4



Compounds of carbon:

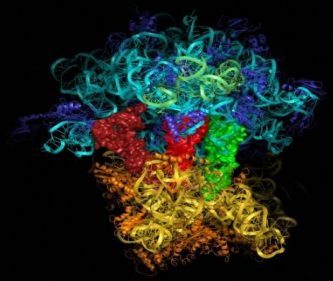
- ethane, C_2H_6
- ethene (ethylene), C_2H_4
- ethyne (acetylene), C_2H_2
- propane. C_3H_8
- butane, C_4H_{10}



Modeling Lab

Conclusion

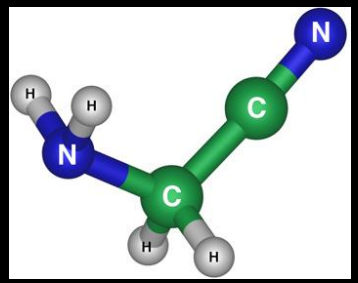
Summarize the different types of bonds studied during this experiment.
How are ionic bonds different from covalent bonds?
What types of geometries did you encounter?

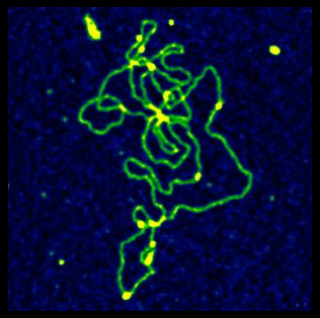


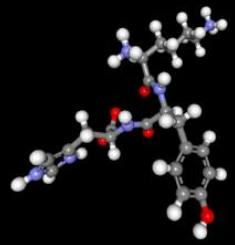
Elementary Modeling Site: (Optional)

Allows Real-time manipulation of simple molecules

http://www-personal.umich.edu/~lpt/Modeling/lab15.htm

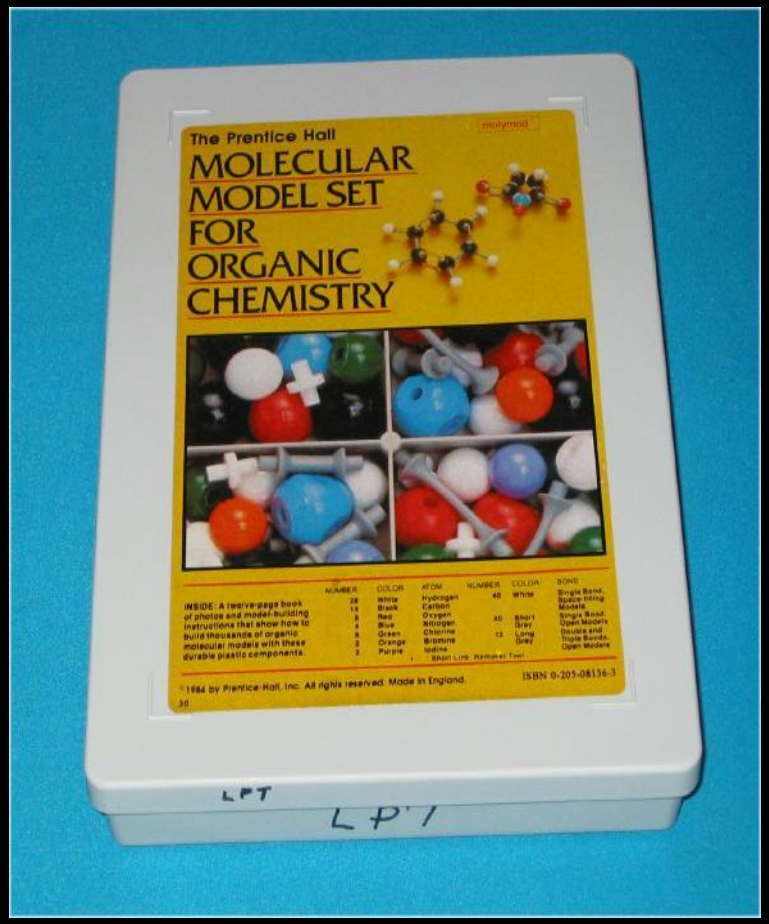


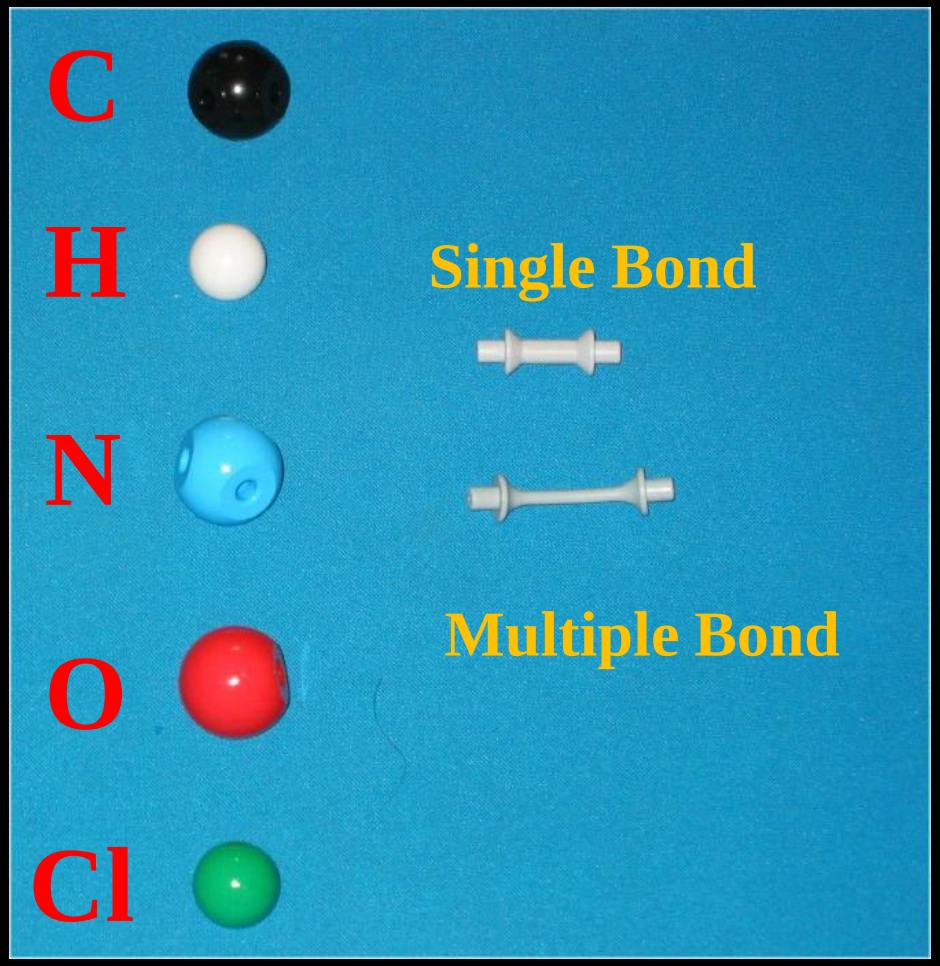




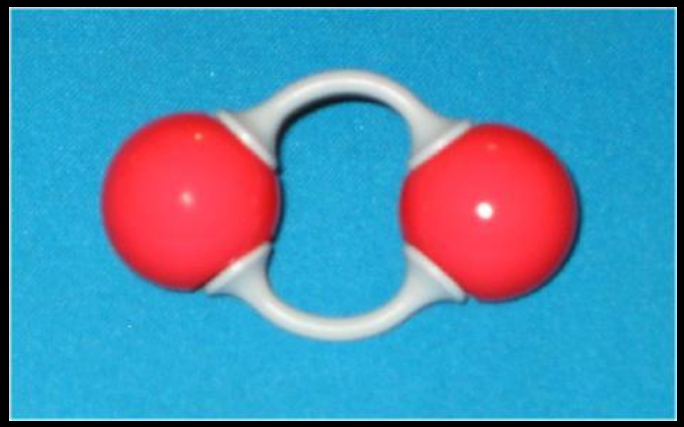
Let’s Boldly Go Explore Today’s Lab

Using the Prentice-Hall Molecular Modeling Set





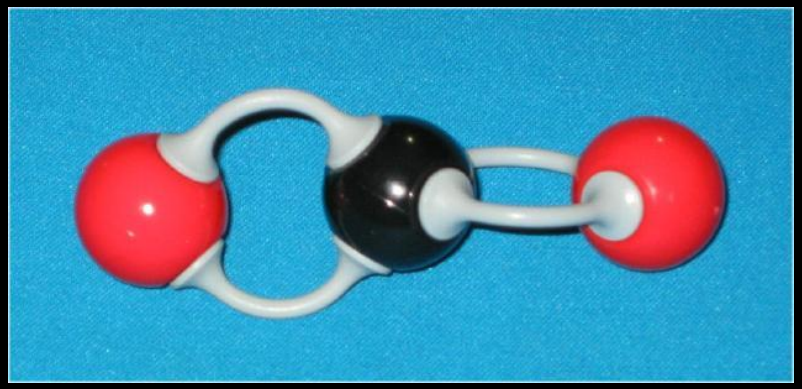
Atmospheric Gases



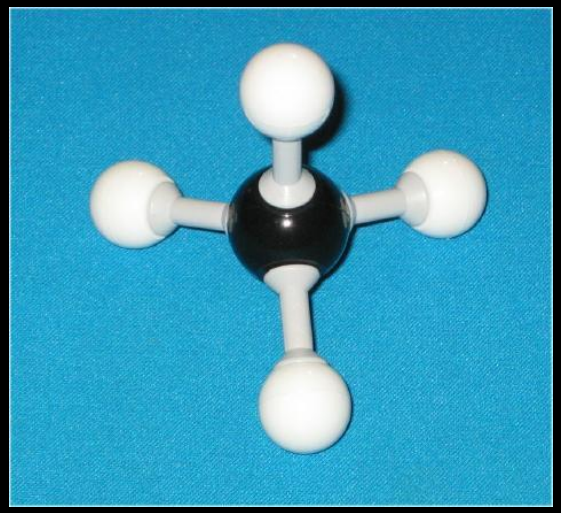
Oxygen: O_2
Linear, Diatomic Molecule
Oxygen - Oxygen Double Bond
(2 Electron Pairs Shared)

Nitrogen: N_2
Linear, Diatomic Molecule
Nitrogen - Nitrogen Triple Bond
(3 Electron Pairs Shared)

Greenhouse Gases

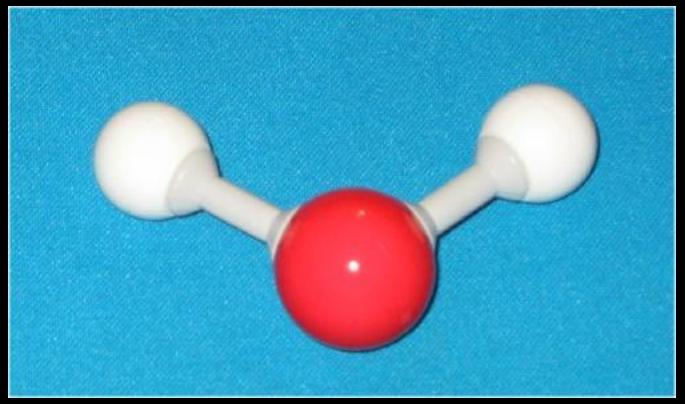


Carbon Dioxide: CO_2
Linear
2 Carbon - Oxygen Double Bonds
Carbon Shares 4 Electron Pairs
Polar Covalent Bonding



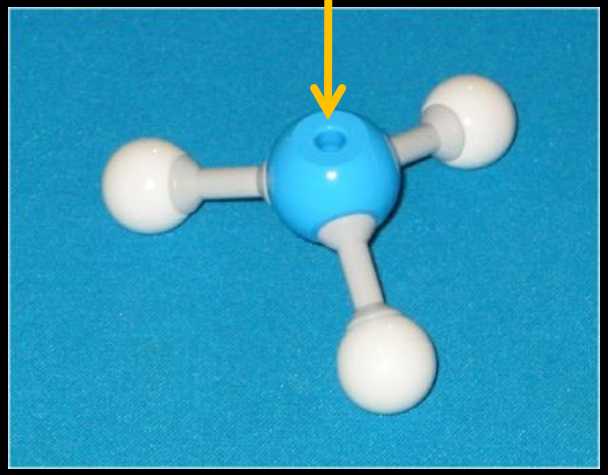
Methane: CH_4
Tetrahedral
4 Carbon - Hydrogen Single Bonds
Carbon Shares 4 Electron Pairs
Non-Polar Covalent Bonding

Others



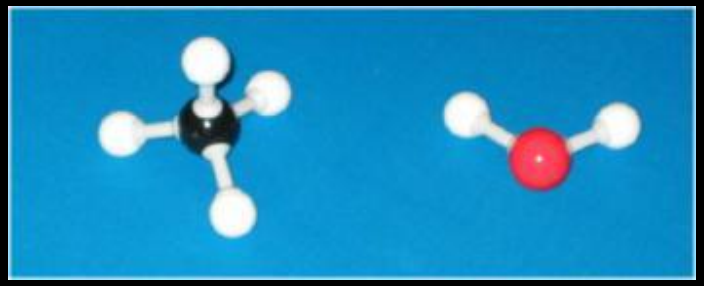
Water: H_2O
2 Lone Pairs Distort Linear Geometry
2 Oxygen Hydrogen Single Bonds
2 Polar Covalent Bonds
Oxygen Shares 2 Electron Pairs

Unshared Pair Occupies this Slot



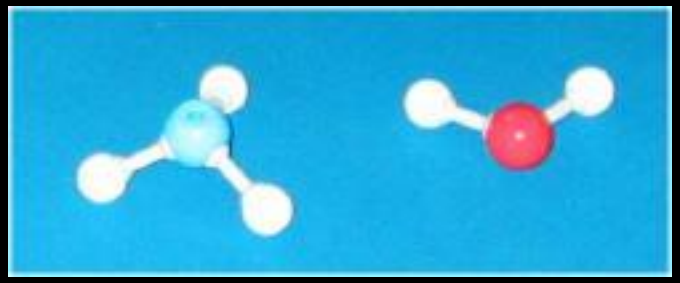
Ammonia: NH_3
3 Nitrogen Hydrogen Single Bonds
3 Non-Polar Covalent Bonds
Nitrogen Shares 3 Electron Pairs
Molecule Has Trigonal-Pyramidal Shape
Unshared Pair Creates Tetrahedral Geometry
(gives molecule a dipole moment)

Models Explain/Predict Molecular Behavior



Methane Compared To Water

Methane is totally symmetrical and non-polar
Water is non-symmetrical and polar
They will not mix



Ammonia Compared To Water

Ammonia has a dipole moment because of 1 unshared electron pair
Water has a dipole moment because of oxygen's 2 unshared pairs of electrons
They will mix

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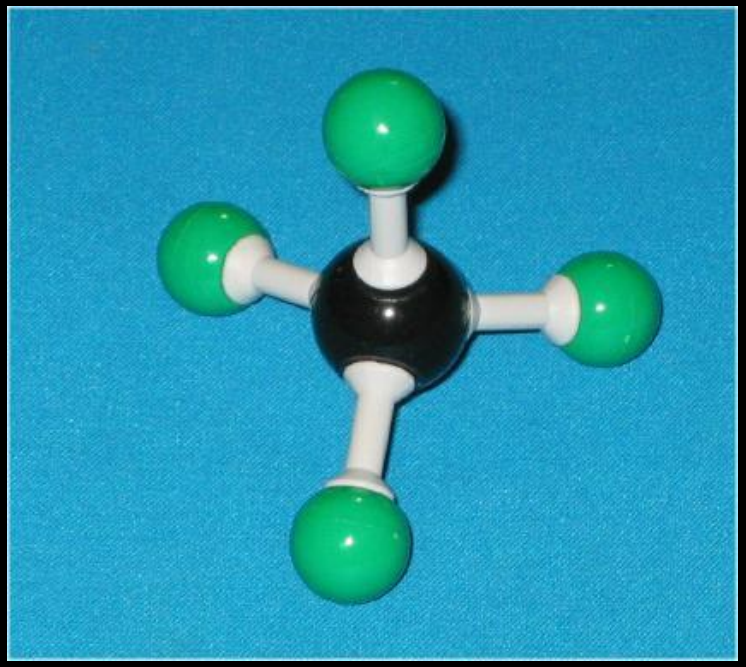
Others

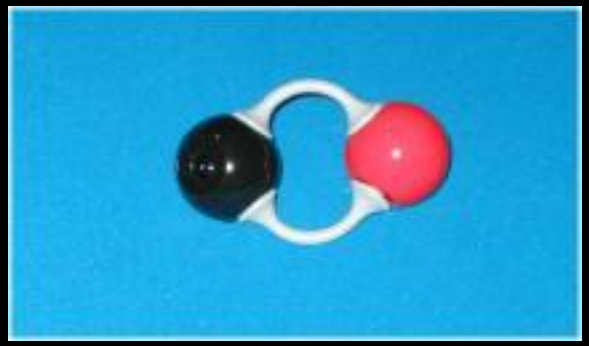


Carbon Tetrachloride: CCl_4
Tetrahedral
4 Carbon - Chlorine Single Bonds
Carbon Shares 4 Electron Pairs
4 Polar Covalent Bonds

Molecule is non-polar
symmetrical
no dipole

Will not mix with water

Molecule With Rendering Problem

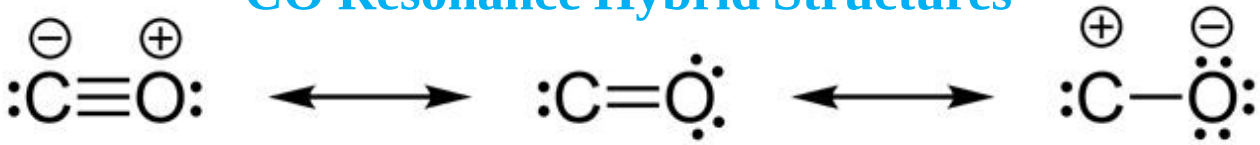


Carbon Monoxide: CO
Linear, Diatomic Molecule
Simple P - H Models Cannot Render
Oxygen: 2 Bonding Sites filled
Carbon: 2 Bonding Sites Empty

CO Molecule Explained By Quantum Mechanical Orbital Mixing (Hybridized Orbitals)

Orbital Electrons "Resonate" (Diffuse and simultaneously occupy several regions)
None of the representations below exist (can be isolated) …
provide visualization of potential mixing of multiple bonding scenarios

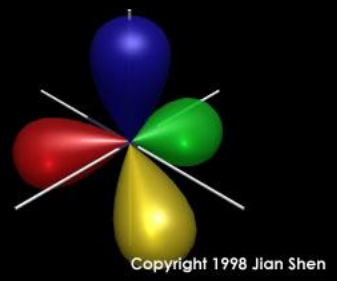
CO Resonance Hybrid Structures

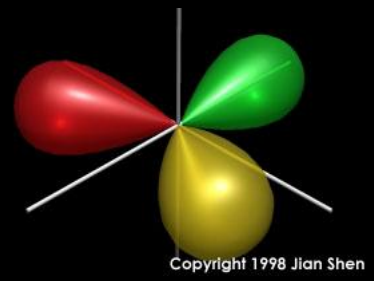


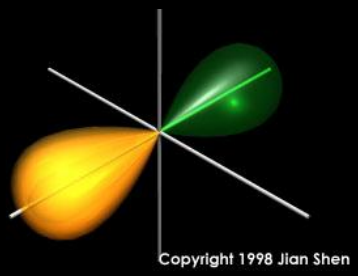
Hybridized Orbitals & Resonance Discussed in Higher Level Classes

Failure Of Lewis Dot & Simple Models To Represent Bonding & Geometry of Many Molecules Led To:

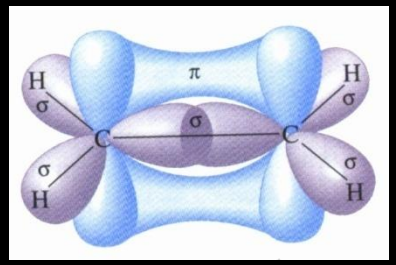
Orbital Mixing



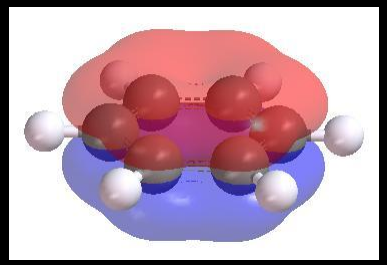




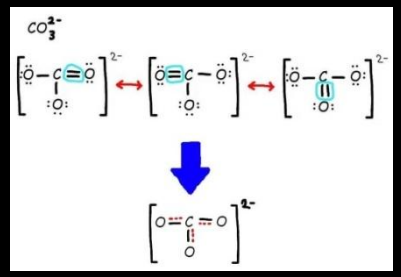
Hybrid Orbitals



Aromaticity



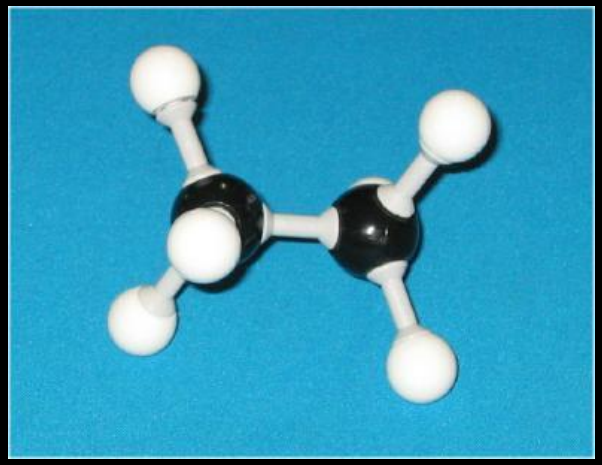
Resonance Structures



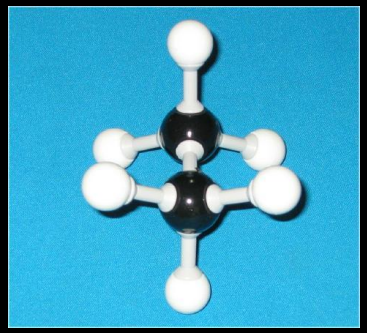
If model fails to explain data, science revises the model

These topics are beyond 101 level

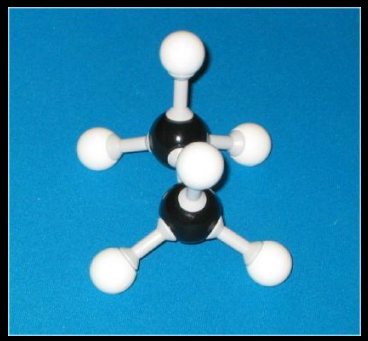
Simple Organic (Carbon-Containing) Molecules



Ethane: C_2H_6
A Hydrocarbon (contains only C and H)
Saturated (all single bonds)
Free Rotation around C - C Bond
6 Non-Polar Covalent C - H Bonds
1 Non-Polar Covalent C - C Bond

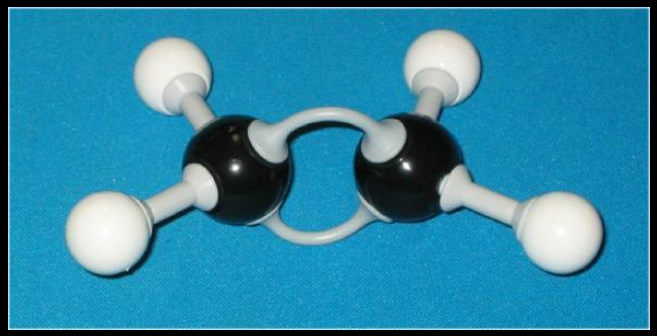


Ethane: C_2H_6
The 2 Methyl Groups (CH_3) are "staggered"



Ethane: C_2H_6
The 2 Methyl Groups (CH_3) are "eclipsed"

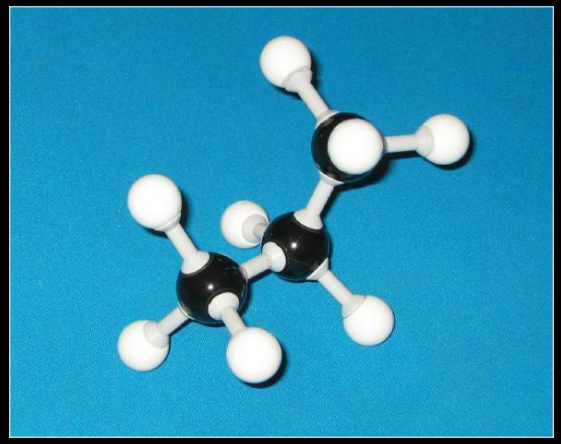
Simple Organic (Carbon-Containing) Molecules



Ethylene (Ethene): C_2H_4
A Hydrocarbon (contains only C and H)
Unsaturated (Contain non-single bond)
No Free Rotation around C - C Double Bond
4 Non-Polar Covalent C - H Bonds
1 Non-Polar Covalent C - C Double Bond
Molecule is planar

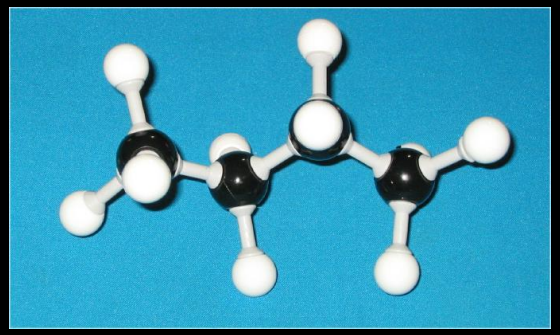
Acetylene (Ethyne) : C_2H_2
A Hydrocarbon (contains only C and H)
Unsaturated (Contain non - single bond)
No Free Rotation around C - C Triple Bond
2 Non-Polar Covalent C - H Bonds
1 Non-Polar Covalent C - C Triple Bond
Molecule is linear

Simple Organic (Carbon-Containing) Molecules



Propane: C_3H_8

A Hydrocarbon (contains only C and H)
Saturated (all single bonds)
Free Rotation around 2 C - C Bonds
8 Non-Polar Covalent C - H Bonds
2 Non-Polar Covalent C - C Bond



Butane: C_4H_{10}

A Hydrocarbon (contains only C and H)
Saturated (all single bonds)
Free Rotation around 3 C - C Bonds
10 Non-Polar Covalent C - H Bonds
3 Non-Polar Covalent C - C Bond

Lab 15 Questions

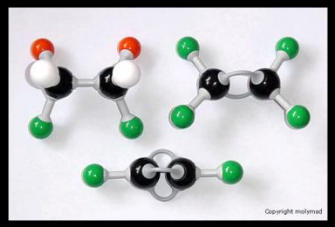
Do the covalent molecules exist as independent units? Explain.

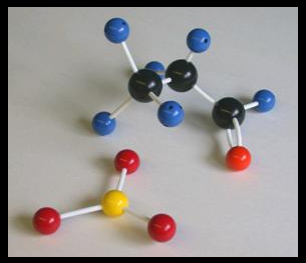
Yes, because they are not ionic matrix compounds.

List the advantages / disadvantages of using ball-and-stick models.

Visualize shape
Evaluate Bonding
Compare different molecules

Difficult for large molecules
May not accurately represent "resonance"
Cost





Based on electronegativity, predict the type of bond for:

Na-Cl

Na = 0.9 Δ = 2.1 Ionic

Cl = 3.0

C-Cl

C = 2.5 Δ = 0.5 Polar Covalent

Cl = 3.0

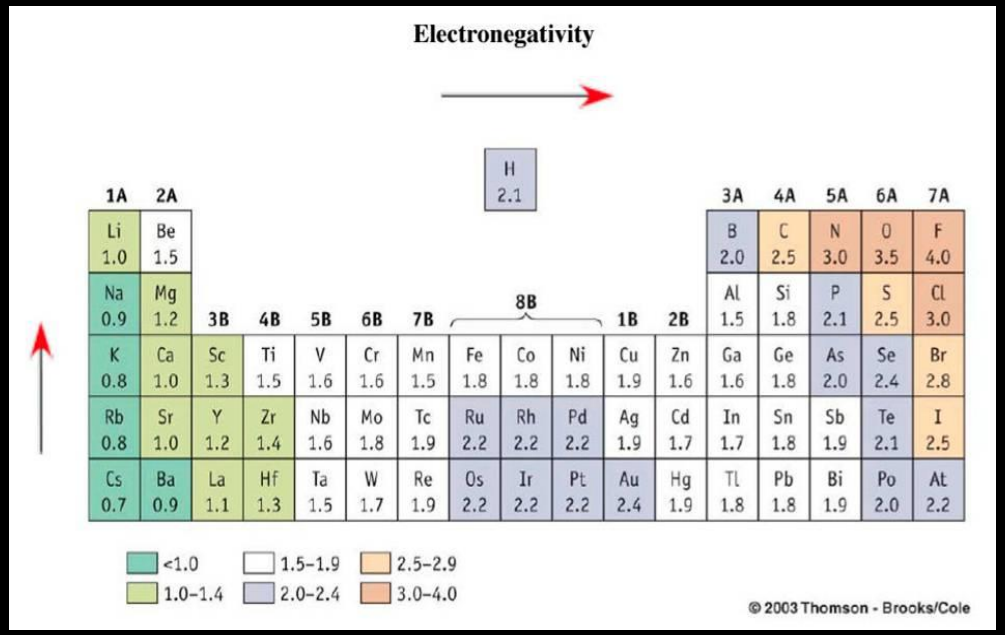
S-O

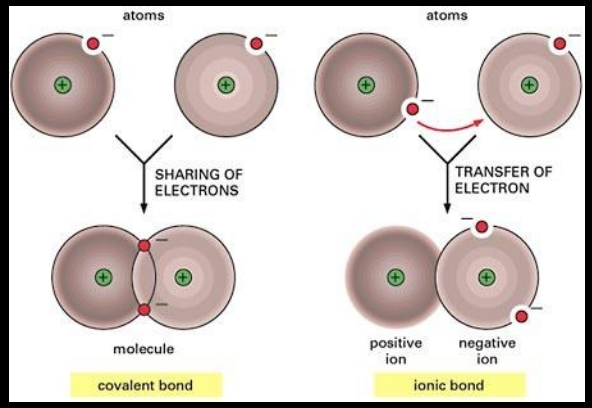
S = 2.5 Δ = 1.0 Polar Covalent

O = 3.5

N-N Δ = 0.0 Non-Polar Covalent

N = 3.0





Δ ≤ 0.4 ➔ non-polar covalent

Δ < 0.4 – 1.9 ➔ polar covalent

Δ > 1.9 ➔ ionic

LPT

Which bond is least polar? Which bond is most polar?

H—O H—S H—P H—C

$\Delta \leq 0.4$ ➔ non-polar covalent
$\Delta < 0.4 – 1.9$ ➔ polar covalent
$\Delta > 1.9$ ➔ ionic

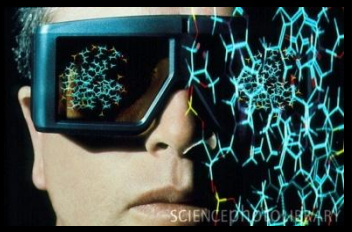
H = 2.1	H = 2.1	H = 2.1	H = 2.1
O = 3.5	S = 2.5	P = 2.1	C = 2.5
Δ ➔ 1.4	Δ ➔ 0.4	Δ ➔ 0.0	Δ = 0.4

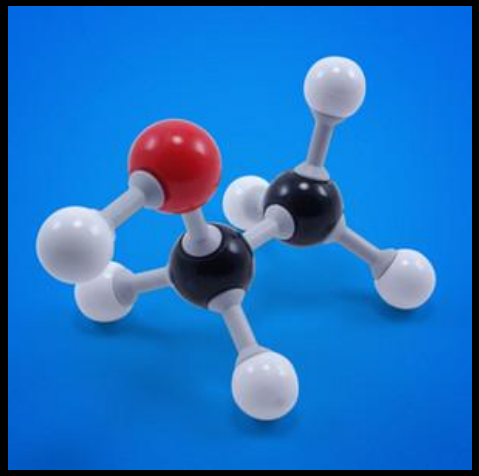
H-P < H-C < H-S < H-O

H-P least polar
H-O most polar

Most Polar of all

Chemistry is a 3D Process
Molecular Models Facilitate Understanding of Chemical Properties and Reactions





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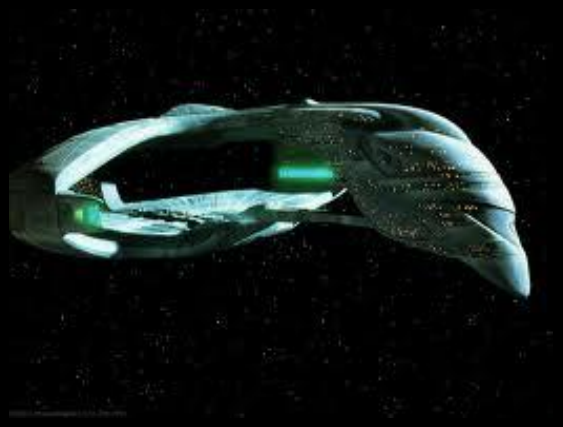
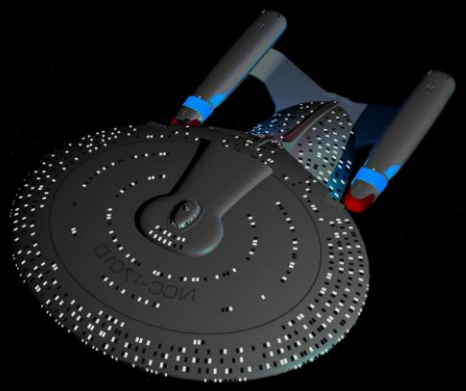




Last Thoughts

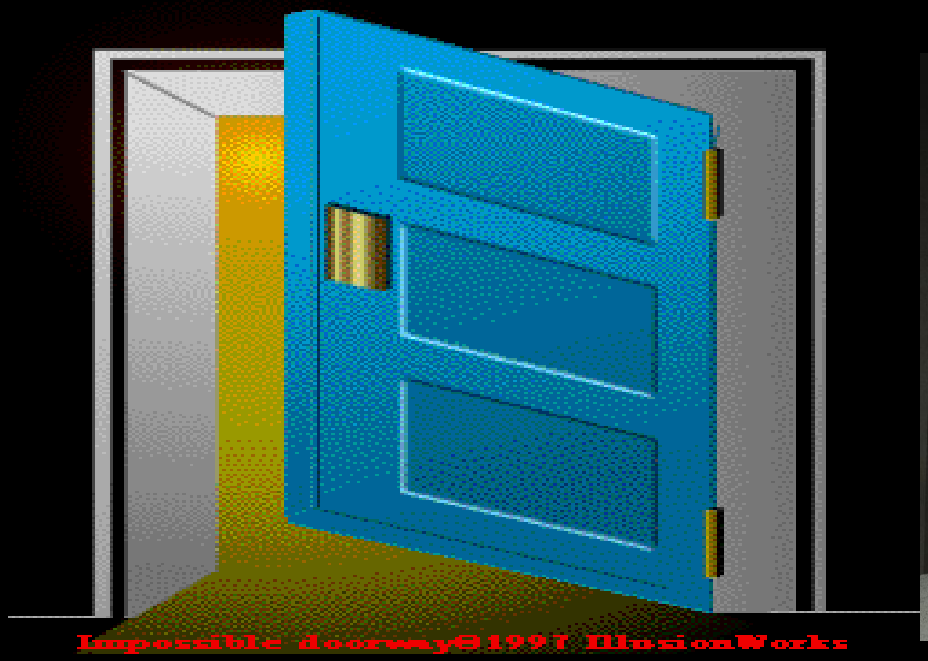
Louis Pasteur

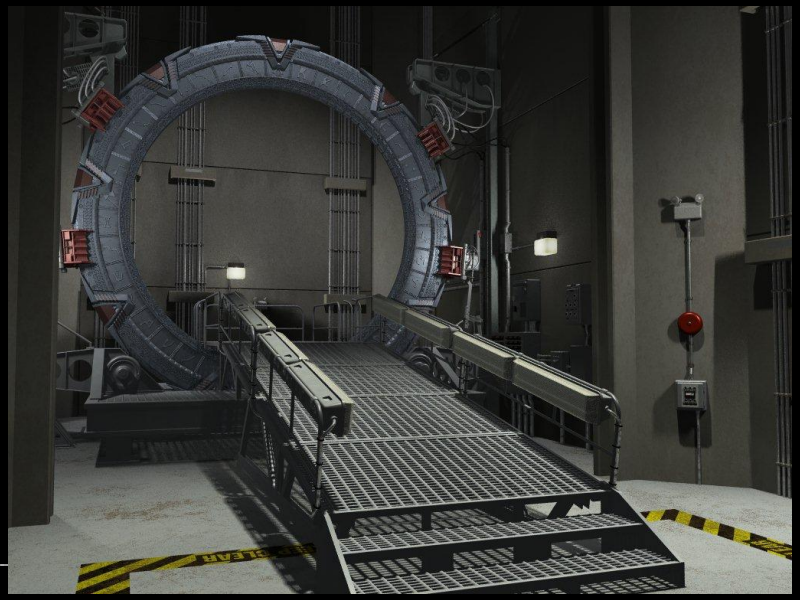
Mid-1800's

Promoted germ theory of disease
Developed Pasteurization process
Debunked spontaneous generation of life
Developed cure for anthrax & rabies
Discovered stereoisomers using polarized light

Chance Favors the Prepared Mind

The more
Acquired knowledge
The Greater Your Skill Set
The More Doors Will Open For You





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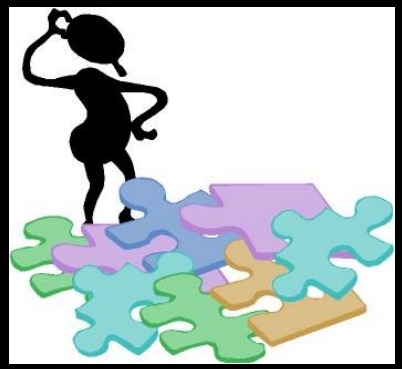


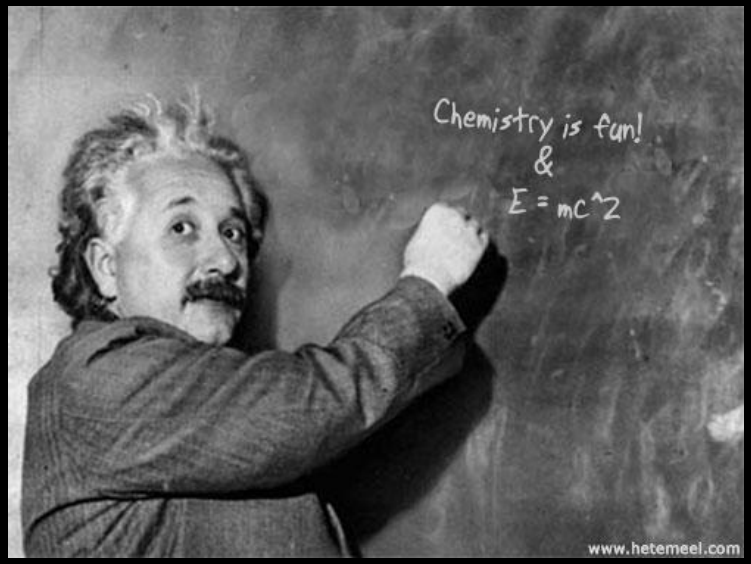
Hopefully

Problems Solving

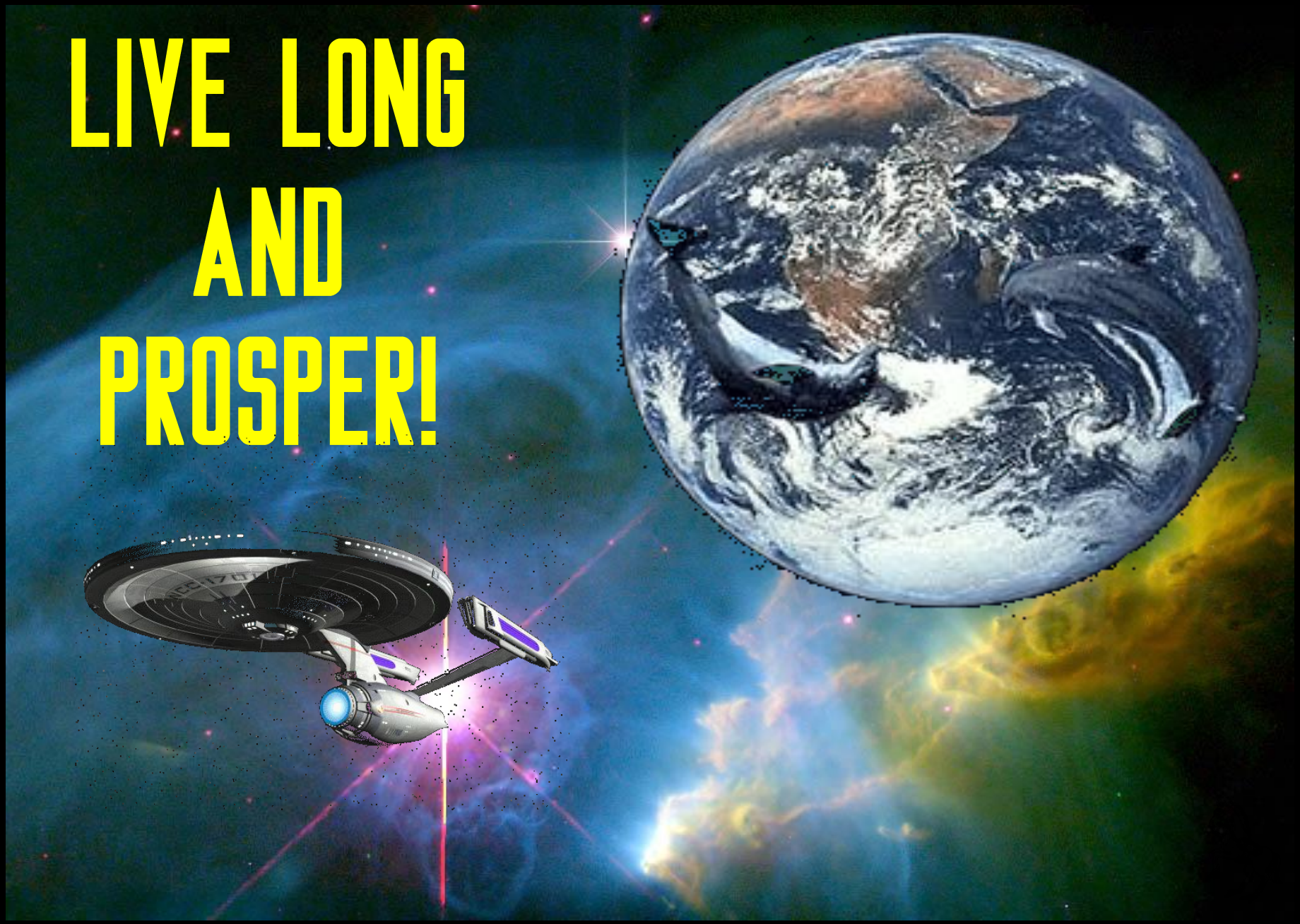
What is the nature of the problem? (Needed)

What do I know (Given)?

How do I get from Known to Needed?



Will stay with you long after memories of this class have faded



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