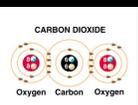
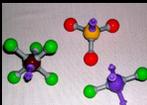


## Chemical Bonds & Modeling



CARBON DIOXIDE  
Oxygen Carbon Oxygen




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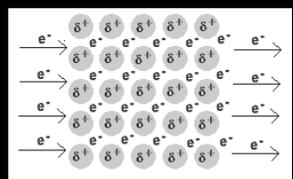
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## Metallic Bonding



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




Explains current flow

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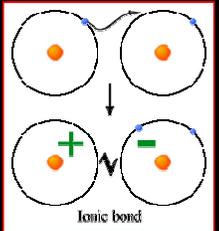
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## Ionic Interactions

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



Ionic bond

**Bond...**  
**Ionic Bond**

“Taken,  
not shared!”



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## Ionic Interactions

**Atoms gain/lose electrons to mutually become "Noble"**

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## Gain or Lose Electrons?

Metals → lose electrons  
Non-Metals → gain or share

**Metals: Alkali metals, Alkaline Earth metals, Transition metals, Other metals**

**Non-metals: Semi-metals, Halogens, Noble gases, Other non-metals**

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## Covalent Bonding

Atoms share electrons to complete "Octet"

Two valence electrons are shared. This gives each Fluorine atom an octet in the valence shell

Happy fluorine atom      Happy fluorine atom

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### Electronegativity Differences

$\Delta \leq 0.4 \rightarrow$  non-polar covalent  
 $\Delta > 0.4 - 1.9 \rightarrow$  polar covalent  
 $\Delta > 1.9 \rightarrow$  ionic  
 $\Delta =$  difference in electronegativity of the bonded atoms



1A		2A		3A										4A										5A										6A										7A																									
Li	1.0	Be	1.5	B	2.0	C	2.5	N	3.0	O	3.5	F	4.0	Al	1.5	Si	1.8	P	2.1	S	2.5	Cl	3.0	Br	2.8	I	2.5	Na	0.9	Mg	1.2	Ca	1.0	Sr	1.0	Ba	0.9	Rb	0.8	K	0.8	Li	1.0	Be	1.5	B	2.0	C	2.5	N	3.0	O	3.5	F	4.0	Al	1.5	Si	1.8	P	2.1	S	2.5	Cl	3.0	Br	2.8	I	2.5

Legend: 
 ■  $\leq 1.0$     ■ 1.0-1.4    ■ 1.5-1.9    ■ 2.0-2.4    ■ 2.5-2.9    ■ 3.0-4.0

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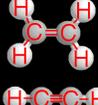
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### Multiple Bonding

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



$:\ddot{\text{N}}\cdot + \cdot\ddot{\text{N}}: \rightarrow :\text{N}:::\text{N}:$   
 $(:\text{N} \equiv \text{N}:)$

$\text{O}=\text{O}$      $\text{O}=\text{O}$   
  
 $\text{H}_2\text{C}=\text{CH}_2$      $\text{H}-\text{C} \equiv \text{C}-\text{H}$



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### Central Atom Bonding Determines Molecular Shape

Number of electron bonding groups:

2                    3                    4                    5                    6

Linear	Trigonal-planar	Tetrahedral	Trigonal-bipyramidal	Octahedral
				
$180^\circ$	$120^\circ$	$109.5^\circ$	$120^\circ$ / $90^\circ$	$90^\circ$
$\text{AX}_2$ Example: $\text{BeF}_2$	$\text{AX}_3$ Example: $\text{BF}_3$	$\text{AX}_4$ Example: $\text{CF}_4$	$\text{AX}_5$ Example: $\text{PF}_5$	$\text{AX}_6$ Example: $\text{SF}_6$

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### Lone Pair Repulsion Finalizes Shape

# Groups	Bond angles	Spatial geometry	Electron pair geometry	Lone pair substitutions
2	180°	Linear	(sp)	Linear
3	120°	Trigonal planar	(sp <sup>2</sup> )	Bent
4	109.5°	Tetrahedral	(sp <sup>3</sup> )	Bent, Trigonal pyramidal
5	90°, 120°	Trigonal bipyramidal	(sp <sup>3</sup> d)	"See-saw", T-shaped, Linear
6	90°	Octahedral	(sp <sup>3</sup> d <sup>2</sup> )	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

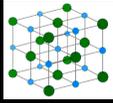
#### Create a data table

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<sup>+</sup> to Cl<sup>-</sup> ions? (1:1)



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### 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.



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### Construct each of the following models

The gases in air:

oxygen, O<sub>2</sub>

nitrogen, N<sub>2</sub>

The "greenhouse gases"

carbon dioxide, CO<sub>2</sub>

methane, CH<sub>4</sub>

Others:

water, H<sub>2</sub>O

ammonia, NH<sub>3</sub>

carbon tetrachloride, CCl<sub>4</sub>

Compounds of carbon:

ethane, C<sub>2</sub>H<sub>6</sub>

ethene (ethylene), C<sub>2</sub>H<sub>4</sub>

ethyne (acetylene), C<sub>2</sub>H<sub>2</sub>

propane, C<sub>3</sub>H<sub>8</sub>

butane, C<sub>4</sub>H<sub>10</sub>



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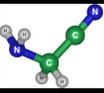
## Modeling Lab




**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>





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## Let's Boldly Go Explore Today's Lab



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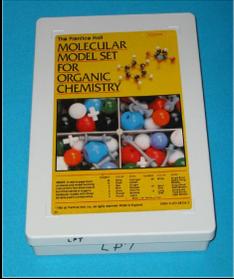
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## Using the Prentice-Hall Molecular Modeling Set



C		
H		Single Bond
		
N		
		
O		Multiple Bond
Cl		

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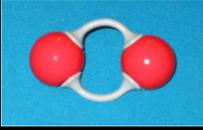
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## Atmospheric Gases



**Oxygen: O<sub>2</sub>**  
Linear, Diatomic Molecule  
Oxygen - Oxygen Double Bond  
(2 Electron Pairs Shared)



**Nitrogen: N<sub>2</sub>**  
Linear, Diatomic Molecule  
Nitrogen - Nitrogen Triple Bond  
(3 Electron Pairs Shared)

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## Greenhouse Gases



**Carbon Dioxide: CO<sub>2</sub>**  
Linear  
2 Carbon - Oxygen Double Bonds  
Carbon Shares 4 Electron Pairs  
Polar Covalent Bonding



**Methane: CH<sub>4</sub>**  
Tetrahedral  
4 Carbon - Hydrogen Single Bonds  
Carbon Shares 4 Electron Pairs  
Non-Polar Covalent Bonding

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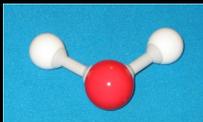
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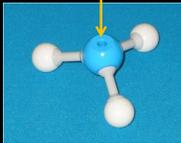
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## Others



**Water: H<sub>2</sub>O**  
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<sub>3</sub>**  
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)

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## 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:  $\text{CCl}_4$   
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

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## Molecule With Rendering Problem



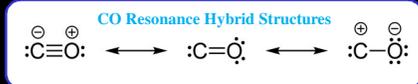
Carbon Monoxide:  $\text{CO}$   
Linear, Diatomic Molecule  
Simple P - H Models Cannot Render  
Oxygen: 2 Bonding Sites filled  
Carbon: 2 Bonding Sites Empty

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



Hybridized Orbitals & Resonance Discussed in Higher Level Classes

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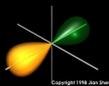
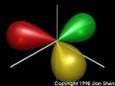
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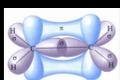
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## Failure Of Lewis Dot & Simple Models To Represent Bonding & Geometry of Many Molecules Led To:

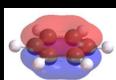
### Orbital Mixing



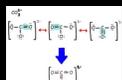
### Hybrid Orbitals



### Aromaticity



### Resonance Structures



If model fails to explain data, science revises the model  
These topics are beyond 101 level

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## 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"

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## 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

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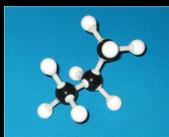
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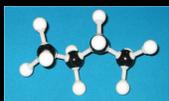
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## Simple Organic (Carbon-Containing) Molecules



**Propane: C<sub>3</sub>H<sub>8</sub>**  
 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<sub>4</sub>H<sub>10</sub>**  
 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

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## Lab 15 Questions

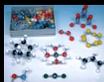
Do the covalent molecules exist as independent units? Explain.

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



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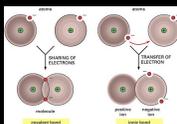
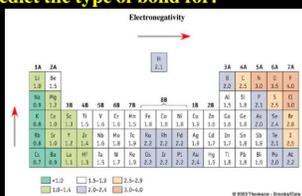
## Based on electronegativity, predict the type of bond for:

**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

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Which bond is least polar? Which bond is most polar?  
 $\text{H}-\text{O}$     $\text{H}-\text{S}$     $\text{H}-\text{P}$     $\text{H}-\text{C}$

$\Delta \leq 0.4$     $\rightarrow$  non-polar covalent  
 $\Delta < 0.4 - 1.9$   $\rightarrow$  polar covalent  
 $\Delta > 1.9$     $\rightarrow$  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
$\Delta \rightarrow 1.4$	$\Delta \rightarrow 0.4$	$\Delta \rightarrow 0.0$	$\Delta = 0.4$

$\text{H}-\text{P} < \text{H}-\text{C} < \text{H}-\text{S} < \text{H}-\text{O}$


**H-P least polar**  
**H-O most polar**





**Most Polar of all**

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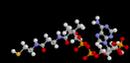
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**Chemistry is a 3D Process**  
**Molecular Models Facilitate Understanding**  
**of Chemical Properties and Reactions**





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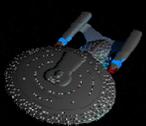
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**Last Thoughts**



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**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**

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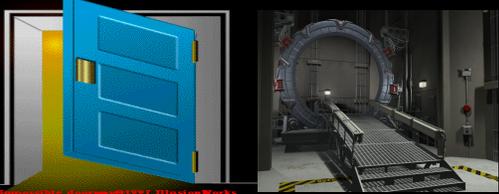
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**The more  
Acquired knowledge  
The Greater Your Skill Set  
The More Doors Will Open For You**



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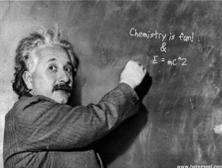
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**Hopefully**

**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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