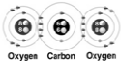
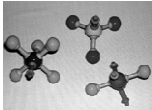
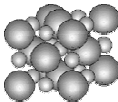


Chemical Bonds & Modeling

CARBON DIOXIDE




Oxygen Carbon Oxygen





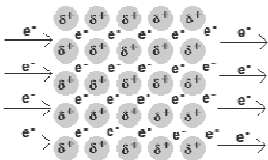
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Metallic Bonding



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






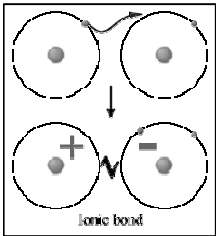
Explains current flow

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Ionic Interactions

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






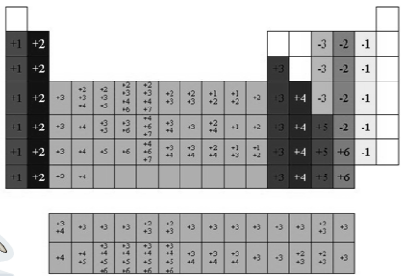
ionic bond




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Ionic Interactions








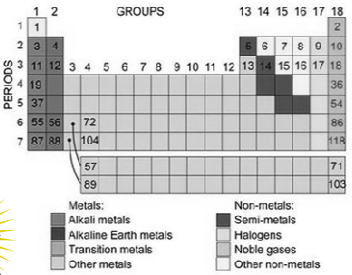
Atoms gain/lose electrons to mutually become “Noble”


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Gain or Lose Electrons?

Metals → lose electrons
Non-Metals → gain or share








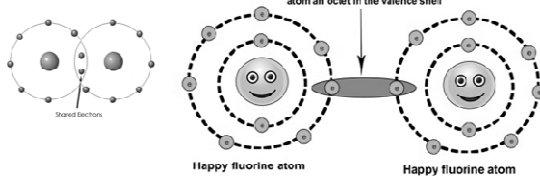
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Covalent Bonding


Atoms share electrons to complete “Octet”



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

Electronegativity

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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

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

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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°	120°	109.5°	120° and 90°	90°
AB_2 Example: BeF_2	AB_3 Example: BF_3	AB_4 Example: CF_4	AB_5 Example: PF_5	AB_6 Example: SF_6

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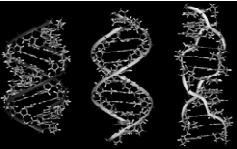
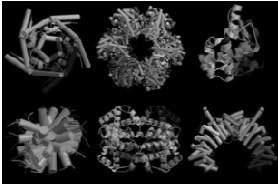
Lone Pair Repulsion Finalizes Shape

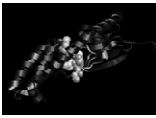

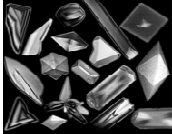
# Groups	Bond angles	Spatial geometry	Electron pair geometry	Lone pair substitutions
2	180°	Linear	(sp)	...
3	120°	Trigonal planar	(sp ²)	Bent
4	109.5°	Tetrahedral	(sp ³)	Trigonal pyramidal, Bent
5	90°, 120°	Trigonal bipyramidal	(sp ³ d)	"See-saw", T-shaped, Linear
6	90°	Octahedral	(sp ³ d ²)	Square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

Maximize distance
Between electron pairs

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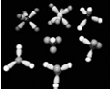
Basic Chemical Theology; Form & Function Intimately Related



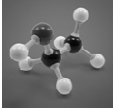



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Modeling Lab

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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

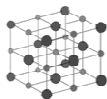
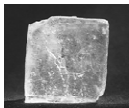
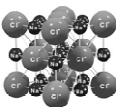
Create a data table

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)



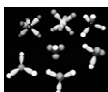
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Making Models (Work in pairs)

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, O₂

nitrogen, N₂

The "greenhouse gases"

carbon dioxide, CO₂

methane, CH₄

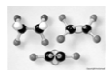


Others:

water, H₂O

ammonia, NH₃

carbon tetrachloride, CCl₄



Compounds of carbon:

ethane, C₂H₆

ethene (ethylene), C₂H₄

ethyne (acetylene), C₂H₂


propane, C₃H₈

butane, C₄H₁₀




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Modeling Lab

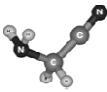

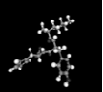


Conclusion

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>

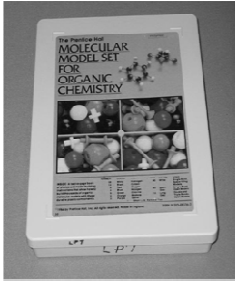
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
Let's Boldly Go Explore Today's Lab





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Using the Prentice-Hall Molecular Modeling Set




C		
H		
N		
O		
Cl		

Single Bond

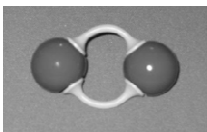


Multiple Bond

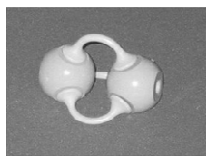


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Atmospheric Gases



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

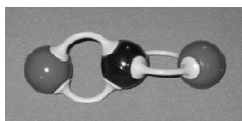


Nitrogen: N_2
Linear, Diatomic Molecule
Nitrogen - Nitrogen Triple Bond
(3 Electron Pairs Shared)

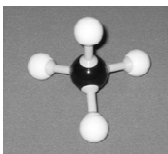
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Greenhouse Gases



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

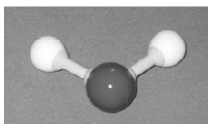


Methane: CH_4
Tetrahedral
4 Carbon - Hydrogen Single Bonds
Carbon Shares 4 Electron Pairs
Non-Polar Covalent Bonding

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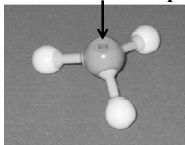
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Others



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

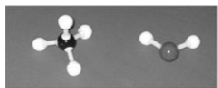


Ammonia: NH_3
3 Nitrogen Hydrogen Single Bonds
3 Non-Polar Covalent Bonds
Nitrogen Shares 3 Electron Pairs
Molecule Has Trigonal-Pyramidal Shape
Unshared Pair Creates Tetrahedral Geometry
(gives molecule a dipole moment)

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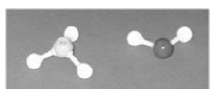
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Models Explain/Predict Molecular Behavior



Methane Compared To Water

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



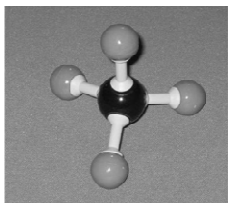
Ammonia Compared To Water

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

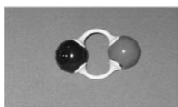
Molecule is non-polar
symmetrical
no dipole

Will not mix with water

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Molecule With Rendering Problem



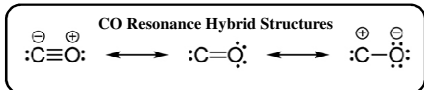
Carbon Monoxide: CO
Linear, Diatomic Molecule
Simple P - H Models Cannot Render
Oxygen: 2 Bonding Sites filled
Carbon: 2 Bonding Sites Empty

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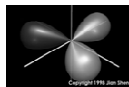
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Failure Of Lewis Dot & Simple Models To Represent Bonding & Geometry of Many Molecules Led To:

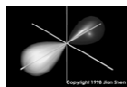
Orbital Mixing



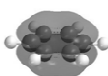
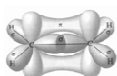
Hybrid Orbitals



Aromaticity



Resonance Structures

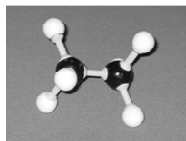


If model fails to explain data, science revises the model
These topics are beyond 101 level

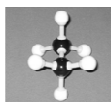
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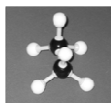
Simple Organic (Carbon-Containing) Molecules



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"

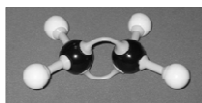


Ethane: C_2H_6
The 2 Methyl Groups (CH_3) are "eclipsed"

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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

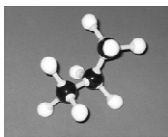


Acetylene (Ethyne) : C_2H_2
A Hydrocarbon (contains only C and H)
Unsaturated (Contain non - single bond)
No Free Rotation around C - C Triple Bond
2 Non-Polar Covalent C - H Bonds
1 Non-Polar Covalent C - C Triple Bond
Molecule is linear

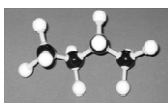
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Simple Organic (Carbon-Containing) Molecules



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

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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

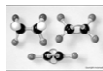
Evaluate Bonding

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 $\Delta = 2.1$ Ionic

Cl = 3.0

C-Cl

C = 2.5 $\Delta = 0.5$ Polar Covalent

Cl = 3.0

S-O

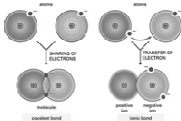
S = 2.5 $\Delta = 1.0$ Polar Covalent

O = 3.5

N-N

$\Delta = 0.0$ Non-Polar Covalent

N = 3.0



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

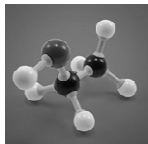
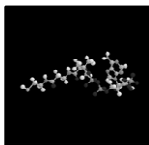


Most Polar of all

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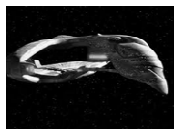
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Chemistry is a 3D Process Molecular Models Facilitate Understanding of Chemical Properties and Reactions



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Last Thoughts



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Louis Pasteur

Mid-1800's

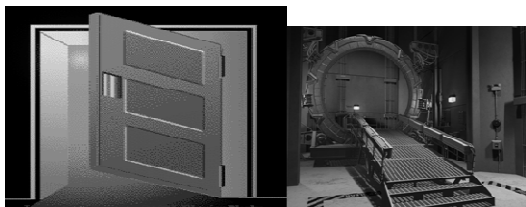
Promoted germ theory of disease
Developed Pasteurization process
Debunked spontaneous generation of life
Developed cure for anthrax & rabies
Discovered stereoisomers using polarized light

Chance Favors the Prepared Mind

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



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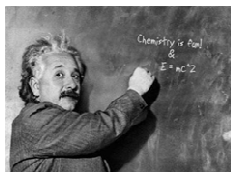
Hopefully

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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