

Chem 108: Lab Week 8

Sign in
Pick up papers
Sit with the same group as last week.

Chemical Reactions

- ☛ Combination (Synthesis)
- ☛ Decomposition
- ☛ Single Displacement
- ☛ Double Displacement
- ☛ Combustion: Oxidation-Reduction
- ☛ Biological Reactions: Enzyme Catalysts

Example: Fermentation

<http://www.piney.com/BabNinkasi.html>

To DO Today Chemical Reactions

With same fermentation partner; Lab Manual pp.44-45

- ☛ Combination (Synthesis)
- ☛ Decomposition
- ☛ Single Displacement
- ☛ Double Displacement
- ☛ Combustion: Oxidation-Reduction
- ☛ Biological Reactions: Enzyme Catalysts

Example: Fermentation pp.61-67

<http://www.piney.com/BabNinkasi.html>

Complete Cover page Today and turn in next week Molecular Modeling

<http://chemconnections.org/general/chem108/Chemistry%20108%20Molecular%20Modeling%20Form%20Fall%202017.pdf>

Molecular Modeling Report Form

These pages replicate the Molecular Model Lab, pp. 90-103, of the Chemistry 108 Experiments Lab Manual. Complete the following modeling related exercises and include the names of all group members, who contributed to the work, on the form.

The first column lists formulas for a number of compounds. The bonding type to be determined for these compounds using differences in their respective electronegativity values (refer to the in class information). The second column is for the electronegativity difference, the absolute value of the difference in electronegativity between the 2 different atoms in the compound. (EN_A - EN_B)². The third column is for the average electronegativity of the two atoms. (EN_A + EN_B) / 2.

Compound	$(EN_A - EN_B)^2$	$\frac{EN_A + EN_B}{2}$	Bonding Type
HF			
HCl			
HBr			
HI			
CF ₄			
NaF			
CaO			
BaO			
NH ₃			
CH ₄			
CCl ₄			
H ₂ O			
NO			
SO ₂			
H ₂			
O ₂			

<http://molview.org>

Molecular Modeling Computational Chemistry

Covalent Bonds: Lewis Structures, Molecular Shapes

Dr. Ron Rusay

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Molecular Modeling Computational Chemistry

Shapes → Lewis Structures Polarity, Solubility, Stereochemistry Smell, Teratogenicity

Dr. Ron Rusay

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https://www.youtube.com/watch?v=Jq_Ca-HKk1g

Shapes of Molecules



View: What is the shape of a molecule?
George Zaidan and Charles Morton

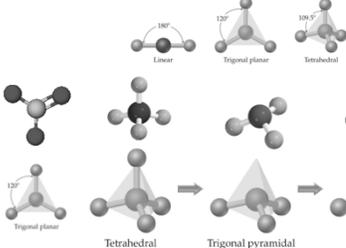


<http://chemconnections.org/general/chem108/Molecular%252520Shapes-Guide.html>

Molecular Shapes

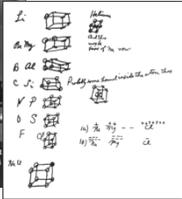
Molecular Models for C, H, N, O

► Fundamental repeating shapes found in every biological molecule



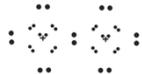
C = black
H = gray
N = blue
O = red
pink = generic atom

Professor Gilbert Newton Lewis (circa 1940)

G.N. Lewis
Photo Bancroft Library, University of California/LBNL Image Library

Footnote:
G.N. Lewis, despite his insight and contributions to chemistry, was never awarded the Nobel prize.



Notes from Lewis's notebook and his "Lewis" structure.

Valence Electrons – Lewis Dot Drawings

A Groups-Periods 2 & 3

	1A(1)	2A(2)	3A(13)	4A(14)	5A(15)	6A(16)	7A(17)	8A(18)
	ns^1	ns^2	ns^2np^1	ns^2np^2	ns^2np^3	ns^2np^4	ns^2np^5	ns^2np^6
Period 2	• Li	• Be •	• B •	• C •	•• N •	•• O •	•• F •	•• Ne ••
Period 3	• Na	• Mg •	• Al •	• Si •	•• P •	•• S •	•• Cl •	•• Ar ••

• H •• C • •• N • •• O •

Covalent Bond Numbers

(Neutral Atoms!)

• H •• F •• •• C • •• N • •• O •

one bond H — F — Cl — Br — I —

two bonds O —
 |

three bonds — N —
 |

four bonds — C —
 |

(Handout)

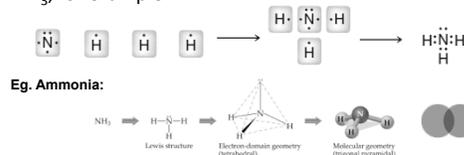
Symbol	Valence electrons	Number of Bonds	Types	Shape	
				electronic	molecular
C	4	4	4 single		
		4	2 single + 1 double		
		4	1 single + 1 triple		
H	1	1	1 single		
O	6	2	1 double		
		2	2 single		
N	5	3	3 single		
		3	1 single + 1 double		
		3	1 triple		

Lewis Structures \longleftrightarrow Molecular Shapes

► For simple Lewis structures:

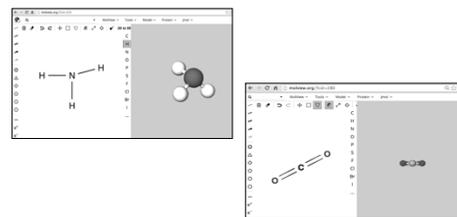
1. Draw the individual atoms using dots to represent the valence electrons.
2. Put the atoms together so they share PAIRS of electrons to make complete octets.

► NH_3 , for example:



<http://molview.org>

Molecular Shapes \longleftrightarrow Lewis Structures MolView: Visual On-line Molecular Modeling



Bonding, Lewis Structures, Molecular Modeling:
Computational Experiments, Instructions, & Manual pp. 53-58

MolView: <http://molview.org/>
<https://www.youtube.com/channel/UCRPSuXCCS9TMgc-kIml34>

Report Form - Molecular Models

Chemical Formula	# Valence e ⁻ s in Molecule	Lewis Structure	Name of VSEPR Arrangement (Molecular Geometry)	Name of Shape (Molecular Geometry)	Bond (Polar or Non-Polar)	Molecule (Polar or Non-Polar)	3 Dimensional Drawing	Resonance (Yes or No)
H_2O								No
NH_3						Polar		No
CH_4								No
C_2H_6			Around each C	Around each C	C-H C-C	Non-Polar		No
HCN			Around C	Around C	H-C C-N	Polar		No
C_2H_2			Around each C	Around each C	C-H C-C			No
SO_2						Non-Polar		Yes

	Orbital (Electronic) Geometry	Molecular Geometry	Bond Angle	# of lone pairs
Important in Organic Compounds	Linear	Linear	180°	0
	Trigonal Planar	Trigonal Planar	120°	0
	Trigonal Planar	Bent	$<120^\circ$	1
	Tetrahedral	Tetrahedral	109.5°	0
	Tetrahedral	Trigonal Pyramidal	$<109.5^\circ$	1
	Tetrahedral	Bent	$<109.5^\circ$	2
See again in Chem 120 and possibly in Chem 109	Trigonal Bipyramidal	Trigonal Bipyramidal	$120^\circ, 90^\circ$	0
	Trigonal Bipyramidal	Seesaw	$<120^\circ, <90^\circ$	1
	Trigonal Bipyramidal	T-shape	$<90^\circ$	2
	Trigonal Bipyramidal	Linear	180°	3
	Octahedral	Octahedral	90°	0
	Octahedral	Square Pyramidal	$<90^\circ$	1
	Octahedral	Square Planar	90°	2

<http://chemconnections.org/general/movies/Lewis%20structures.html>

Covalent Compounds

- Share valence electrons.
- 1 pair = 1 bond; maximum # of atom-atom bonds = 3.
- Octet rule ("duet" for hydrogen)
- Lewis structure examples:

Lewis structures



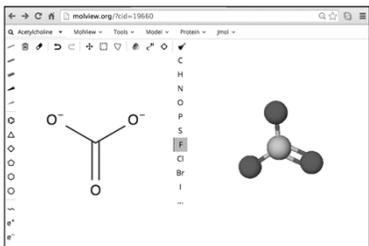
Notice the charges:

In one case they balance, can you name the compound?
In the other they do not.

It has a "Formal" charge. Can you name the polyatomic ion?

<http://molview.org>

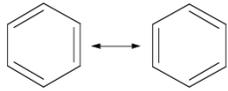
Molecular Shapes \longleftrightarrow Lewis Structures
MolView: Polyatomic Ions



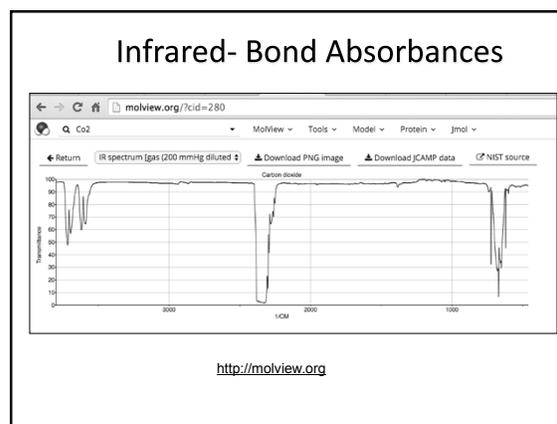
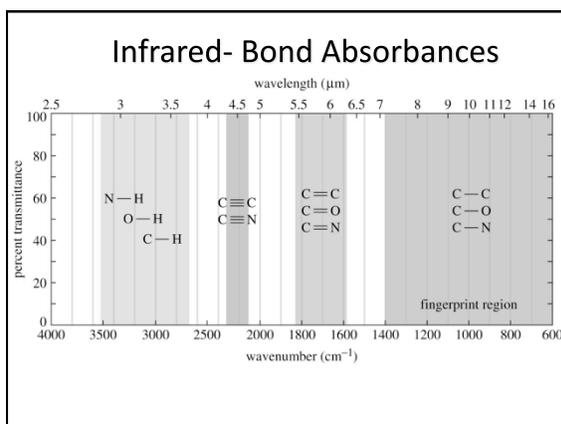
Bonding, Lewis Structures, Molecular Modeling:

Resonance

- Occurs when more than one valid Lewis structure can be written for a particular molecule. [Adjacent free electrons, double or triple bonds.]



- These are resonance structures. The actual structure is an average of all of the resonance structures.



Infrared- Bond Absorbances

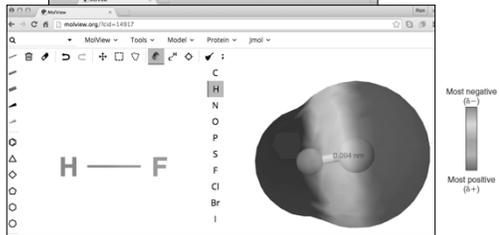
Earth's CO₂ Home Page



<https://www.co2.earth/>

Computational Chemistry

Polarity: Molview (<http://molview.org>) jmol



Color coded electron density distribution: red-highest, blue lowest, green balanced

The more distinct the red-blue colors means the more polar the molecule.

Polarity & Physical Properties Ozone and Water

- Resultant Molecular Dipoles > 0
- Solubility: Polar molecules that dissolve or are dissolved in like molecules

- The Lotus flower
- Water & dirt repellancy: solubility?

Amino Acids Legos of Chemical Biology

Amino acids contain carbon, hydrogen, oxygen, and nitrogen, which resemble the following shapes & structural components

- 20 different amino acids are encoded by the genetic code, which is archived in DNA.
- Hundreds of amino acids link together with amide (peptide) bonds to form proteins, which are the machinery for the chemistry of life.
- There are less than 20,000 total proteins produced from humans' entire genome, each coded by a specific gene in DNA's ~3 billion genetic bases.

Amino Acids → Proteins Indispensable Biopolymers Acetylcholinesterase (ACE)

ACE, an enzyme, which catalyzes a key reaction in a repetitive biochemical cycle that is crucial to neurological and physiological functions in humans.... and insects among others.

4,496 atoms;
4,404 bonds
574 amino acid residues

- starch
- ALPHA & BETA AMYLASE
- sucrose
- INVERTASE
- simple sugars
- ZYMASE
- co2
- alcohol

Biological Reactions eg. Fermentation

<https://www.youtube.com/watch?v=vW99JEaDApY>

<http://www.piney.com/BabNinkasi.html>