Molecular Modeling
Computational Chemistry

http://molview.org

Shapes ⟷ Lewis Structures

Covalent Bonds:
Lewis Structures, Molecular Shapes

Dr. Ron Rusay

https://www.youtube.com/watch?v=Jq_Ca-HKh1g

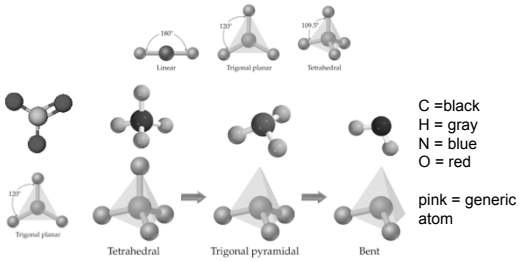
Shapes of Molecules

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

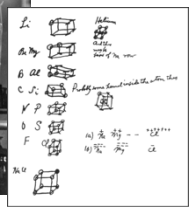
- Fundamental repeating shapes found in every biological and synthetically made organic molecule including plastics



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

Period	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
2	Li	Be	B	C	N	O	F	Ne
3	Na	Mg	Al	Si	P	S	Cl	Ar

Covalent Bond Numbers

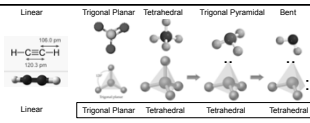
(Neutral Atoms!)

one bond

two bonds

three bonds

four bonds



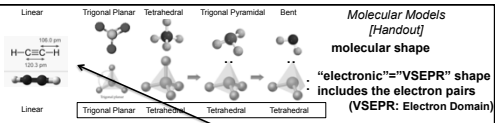
Molecular Models [Handout]

molecular shape

"electronic"="VSEPR" shape includes the electron pairs (VSEPR: Electron Domain)

Symbol	Valence electrons	Number of Bonds	Types	Shape: electronic	Shape: 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		

http://chemconnections.org/general/chem108/Molecular%20Modeling-intro%20%26%20table%202019f.pdf



Molecular Models [Handout]

molecular shape

"electronic"="VSEPR" shape includes the electron pairs (VSEPR: Electron Domain)

Linear = L
Trigonal Planar = TPl
Tetrahedral =T
Trigonal Pyramidal =TPy
Bent = B

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

carbon-carbon bond lengths
Single longest length
Double shorter length
Triple shortest length

http://chemconnections.org/general/chem108/Molecular%20Modeling-intro%20%26%20table%202019f.pdf

http://molview.org

Lewis Structures ↔ Molecular Shapes

Report Form – Molecular Models

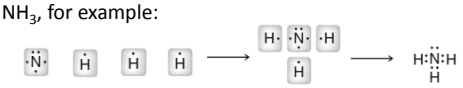
Chemical Formula	# Valence e's in Molecule	Lewis Structure	Name of VSEPR Arrangement (Geometry)	Name of Shape (Molecular Geometry)	Bond (Polar or Non-Polar)	Molecule (Polar or Non-Polar)	3 Dimensional Drawing	Resonance (Yes or No)
H_2O		O H H				Polar		No
NH_3	8	H N H H				Polar		No
CH_4		H C H H H						No
C_2H_4		H C C H H H	Around each C	Around each C	C–H C–C	Non-Polar		No
HCN		H C N	Around C	Around C	H–C C–N	Polar		No
C_2H_2		H C C H	Around each C	Around each C	C–H C–C			No
SO_3		O S O O				Non-Polar		Yes

Name?
Ammonia

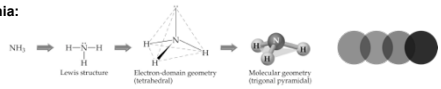
Molecular Modeling: Bonding & Lewis Structures
Computational Chemistry: Molecular Modeling Report Form

Lewis Structures ↔ 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:



Eg. Ammonia:



http://molview.org

Molecular Shapes ↔ Lewis Structures

Report Form – Molecular Models

Chemical Formula	# Valence e's in Molecule	Lewis Structure	Name of VSEPR Arrangement (Geometry)	Name of Shape (Molecular Geometry)	Bond (Polar or Non-Polar)	Molecule (Polar or Non-Polar)	optional 3 Dimensional Drawing	Resonance (Yes or No)
H_2O		O H H				Polar		No
NH_3	8	H–N–H H				Polar		No
CH_4		H C H H H						No
C_2H_4		H C C H H H	Around each C	Around each C	C–H C–C	Non-Polar		No
HCN		H C N	Around C	Around C	H–C C–N	Polar		No
C_2H_2		H C C H	Around each C	Around each C	C–H C–C			No
SO_3		O S O O				Non-Polar		Yes

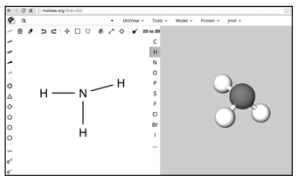
Name?
Ammonia

Molecular Modeling: Bonding & Lewis Structures
Computational Chemistry: Molecular Modeling Report Form

http://molview.org

Molecular Shapes ↔ Lewis Structures

MolView: Visual On-line Molecular Modeling



Bonding, Lewis Structures, Molecular Modeling:
Computational Experiments

http://molview.org

Molecular Shapes ⟷ Lewis Structures

Report Form – Molecular Models

Chemical Formula	# Valence e's in Molecule	Lewis Structure	Name of VSEPR Arrangement (Geometry)	Name of Shape (Molecular Geometry)	Bond (Polar or Non-Polar)	Molecule (Polar or Non-Polar)	optional 3 Dimensional Drawing	Resonance (Yes or No)
H_2O						Polar		No
NH_3	8		Tetra-hedral	Trigonal Planar		Polar		No
CH_4								No
C_2H_4	12					Non-Polar		No
HCN					C–N	Polar		No
C_2H_2			Around each C	Around each C	C–H C–C			No
SO_4						Non-Polar		Yes

Name?
Ammonia

ethylene

Molecular Modeling: Bonding & Lewis Structures
Computational Chemistry: Molecular Modeling Report Form

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Molecular Shapes ⟷ Lewis Structures

Report Form – Molecular Models

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SO_4						Non-Polar		Yes

Name?
Ammonia

ethylene

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Molecular Shapes ⟷ Lewis Structures

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N_2								No
$(NH_4)^+$						Polyatomic Ion		No
PBr_3						Polar		No
$(NO_3)^-$						Polyatomic Ion		Yes
$(CO_3)^{2-}$						Polyatomic Ion		Yes
CH_2O								No

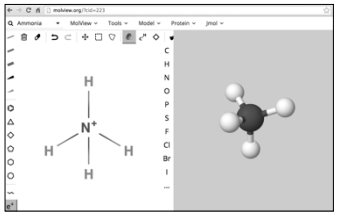
Ammonium

Molecular Modeling: Bonding & Lewis Structures
Computational Chemistry: Molecular Modeling Report Form

http://molview.org

Molecular Shapes ⟷ Lewis Structures

MolView: Visual On-line Molecular Modeling

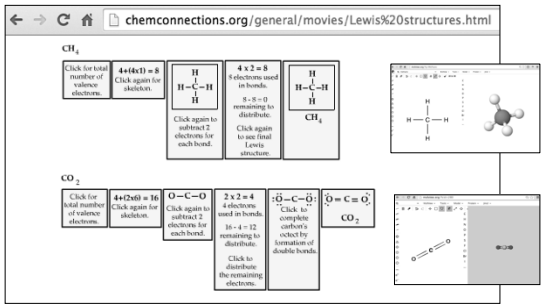


Ammonium (polyatomic ion)

Molecular Modeling: Bonding & Lewis Structures
Computational Chemistry: Molecular Modeling Report Form

	VSEPR (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°	1
	Tetrahedral	Tetrahedral	109.5°	0
	Tetrahedral	Trigonal Pyramidal	<109.5°	1
	Tetrahedral	Bent	<109.5°	2
See again in Chem 120 and possibly in Chem 109	Trigonal Bipyramidal	Trigonal Bipyramidal	120°, 90°	0
	Trigonal Bipyramidal	Seesaw	<120°, <90°	1
	Trigonal Bipyramidal	T-shape	<90°	2
	Trigonal Bipyramidal	Linear	180°	3
	Octahedral	Octahedral	90°	0
	Octahedral	Square Pyramidal	<90°	1
	Octahedral	Square Planar	90°	2

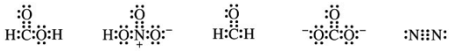
http://chemconnections.org/general/movies/Lewis%20structures.html



Lewis Structures / 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



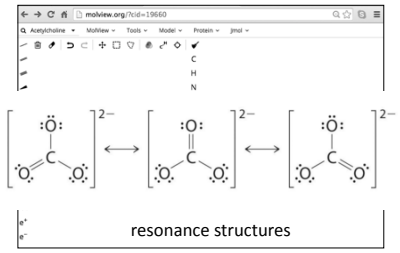
Notice the "formal" charges:
In one case they balance, can you name the compound?
In the other they do not.

They both have "formal" charges. Can you name the polyatomic ion?

http://molview.org

Resonance Models & Lewis Structures

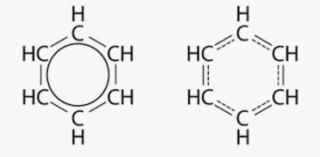
MolView: Carbonate Polyatomic Ion



Bonding, Lewis Structures, Molecular Modeling:

Resonance

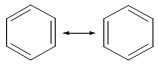
- Occurs when more than one valid Lewis structure can be written for a particular mo double or t



- An overall resonance structure is a weighted average of all of the possible resonance structures.

Question

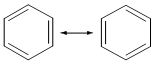
Two resonance structures of benzene, a human carcinogen, with C-C & C=C bonds are shown below. Which statement is incorrect?



A. The double headed arrow indicates that the 2 resonance structures are rapidly interchanging.
B. The normal bond length of a single bond is longer than a double bond.
C. The best resonance structure localizes the bonds so that the double bonds on the right are preferred.
D. The actual bond lengths in benzene are not equal to either single or double bonds.

Answer

Two resonance structures of benzene, a human carcinogen, with C-C & C=C bonds are shown below. Which statement is incorrect?



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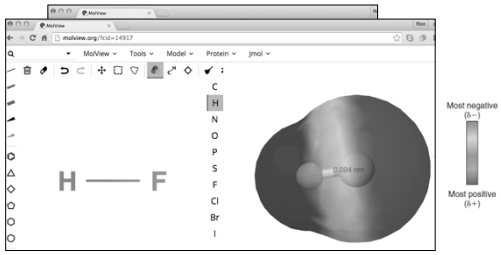
Polarity & Modeling

Polarity: Molview (http://molview.org) Jmol



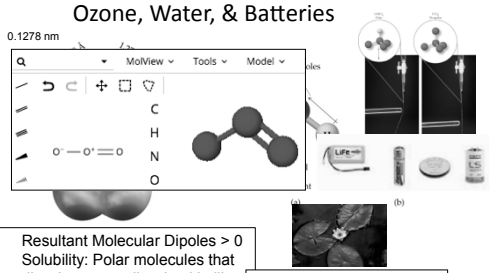
Color coded electron density distribution: red-highest, blue lowest, green balanced

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

https://www.youtube.com/watch?v=ASLUY2U1M-8

Polarity & Physical Properties

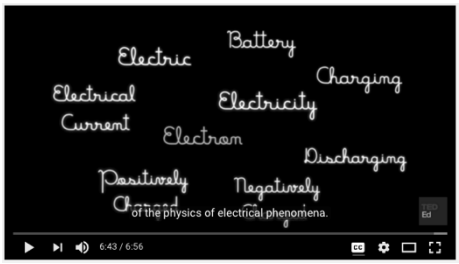
Ozone, Water, & Batteries



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

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

https://www.youtube.com/watch?v=MBRTR2dlwvA&t=244s



http://molview.org

Molecular Shapes⟷ Lewis Structures

Report Form – Molecular Models

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ammonia NH_3	8		Tetra-hedral	Trigonal Planar	Polar	Polar		No
CH_4								No
ethylene C_2H_4	12		Around each C TRIGONAL PLANAR	Around each C TRIG. PLANAR		Non-Polar		No
HCN		H C N			C–N	Polar		No
C_2H_2		H C C H	Around each C	Around each C	C–H C–C			No
SO_3		O S O				Non-Polar		Yes

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Molecular Shapes⟷ Lewis Structures

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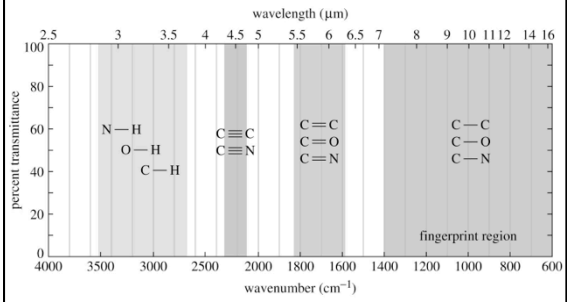
ammonia NH_3	8		Tetra-hedral	Trigonal Planar	Polar	Polar		No
CH_4								No
ethylene C_2H_4	12		Around each C TRIGONAL PLANAR	Around each C TRIG. PLANAR	C-H and also C-C	Non-Polar		No
HCN		H C N			C–N	Polar		No
C_2H_2		H C C H	Around each C	Around each C	C–H C–C			No
SO_3		O S O				Non-Polar		Yes

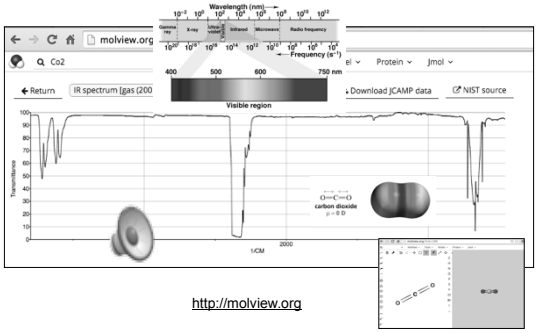
Molecular Modeling: Bonding & Lewis Structures
Computational Chemistry: Molecular Modeling Report Form

Infrared- Bond Absorbances



Invisible Molecular Motions:
https://www.youtube.com/watch?v=b0IbXG0hnOk

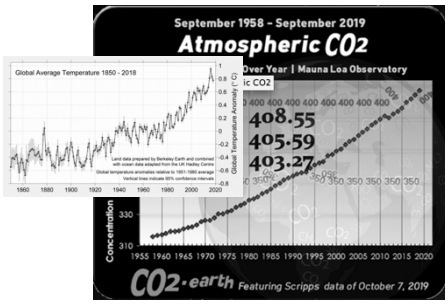
Infrared- Bond Absorbances



http://molview.org

https://www.youtube.com/watch?v=W5gimZlFY6I

Infrared- Bond Absorbances



https://www.co2.earth/