Molecular Modeling
Computational Chemistry

http://molview.org

Shapes ⟶ Lewis Structures

Covalent Bonds:
Lewis Structures, Molecular Shapes

Dr. Ron Rusay

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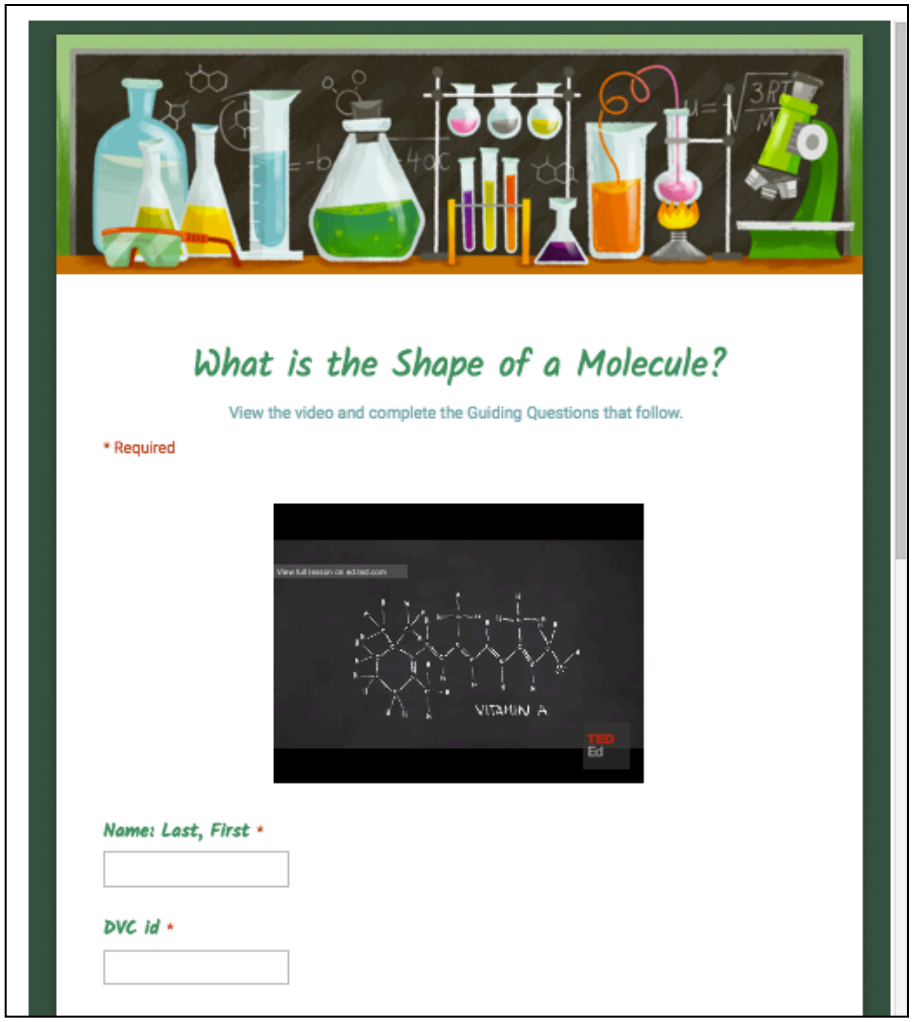
https://www.youtube.com/watch?v=Jq_Ca-HKh1g

Shapes of Molecules

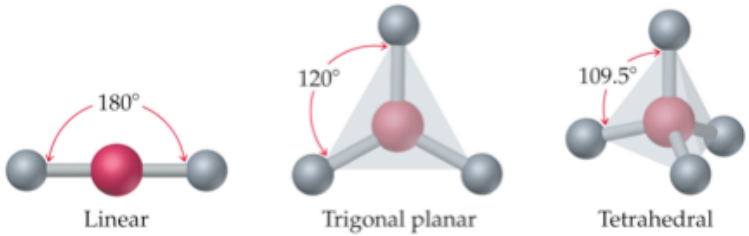


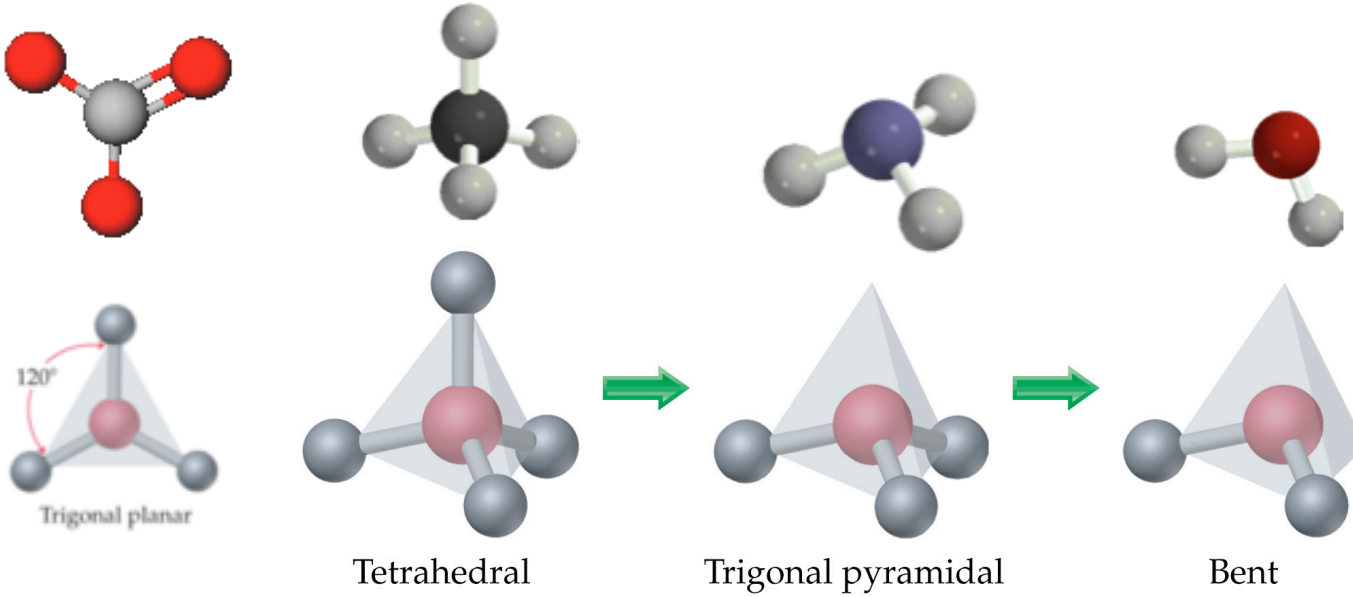
View: What is the shape of a molecule?
George Zaidan and Charles Morton

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

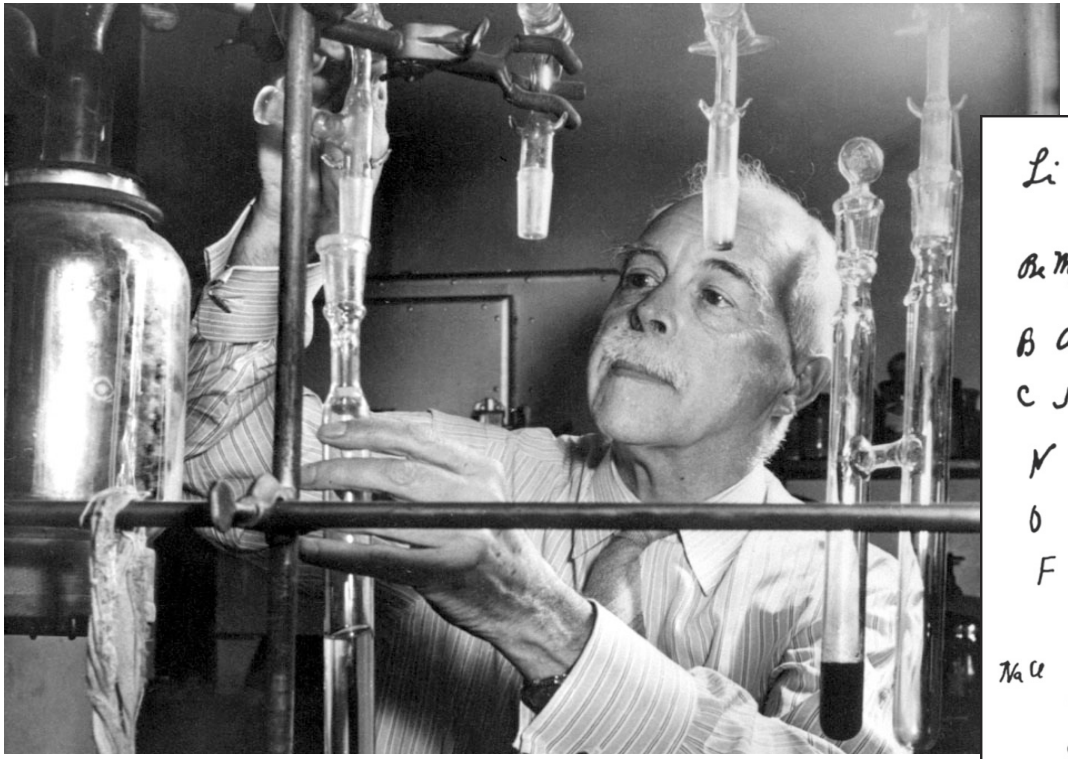


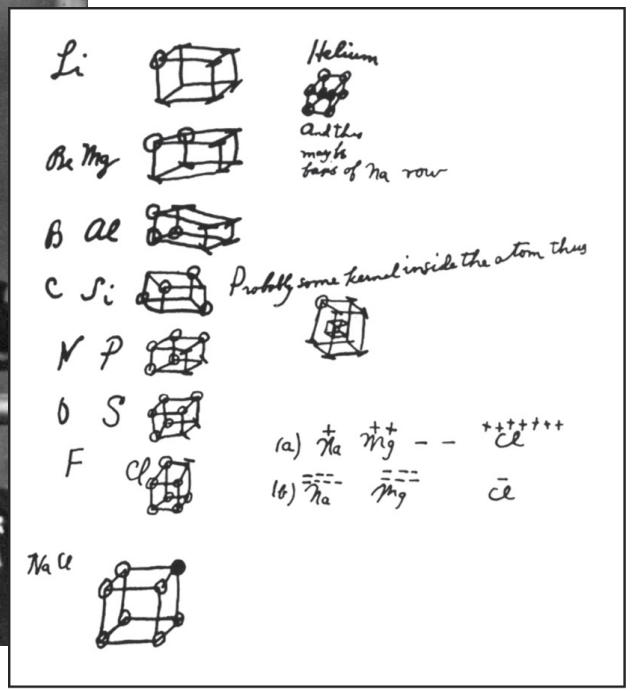


C =black
H = gray
N = blue
O = red

pink = generic atom

Professor Gilbert Newton Lewis (circa 1940)



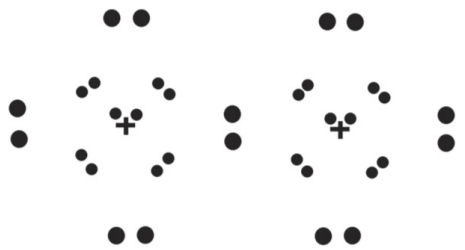


G.N. Lewis

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

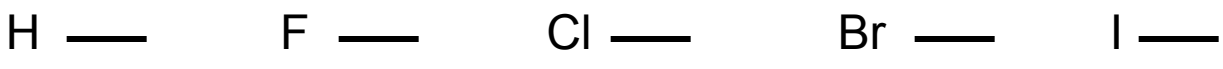
A Groups-Periods 2 & 3

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

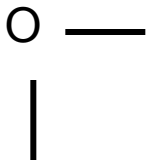
Covalent Bond Numbers

(Neutral Atoms!)

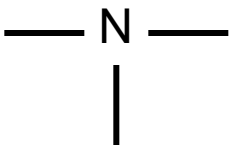
one bond



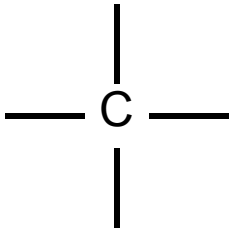
two bonds



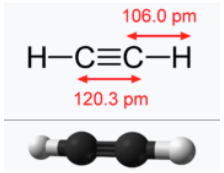
three bonds

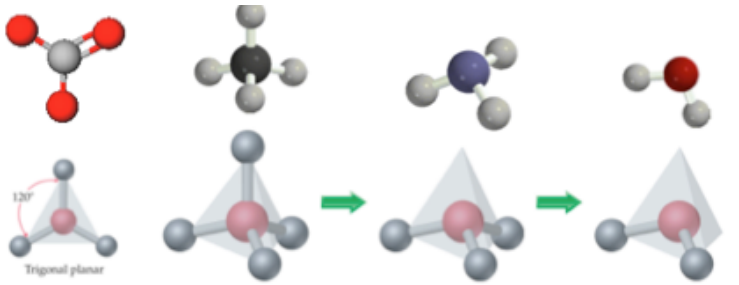


four bonds



Linear Trigonal Planar Tetrahedral Trigonal Pyramidal Bent





Linear Trigonal Planar Tetrahedral Tetrahedral Tetrahedral

molecular shape

electronic shape
(VSEPR: Electron Domain)

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		

(Collaborative)

Names: _____

Molecular Modeling Report Form

These pages replace the Molecular Model Lab, pp. 97-103, 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 is 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, $|EN_2 - EN_1|$. The third column is for the average electronegativity of the two atoms, $(EN_1 + EN_2)/2$.

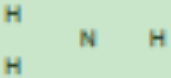
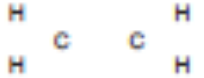
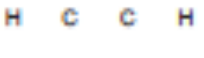
Compound	$\lvert EN_1 - EN_2 \rvert$	$\frac{EN_1 + EN_2}{2}$	Bonding Type
HF	*4.0 – 2.1 = 1.9*	*3.0*	*polar covalent*
HCl			
HBr			
HI			
CsF			
NaF			
CaO			
BaO			
NH_3			
CH_4			
CCl_4			
H_2O			
N_2O			
SO_2			
H_2			
O_2			

http://molview.org

Molecular Shapes → Lewis Structures

Name?
Ammonia

Report Form – Molecular Models

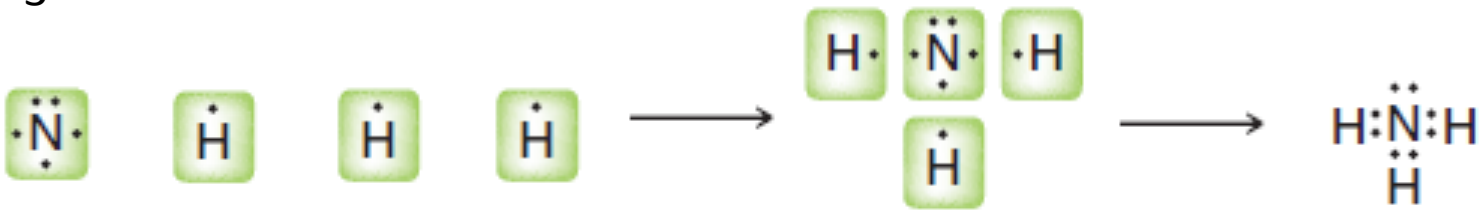
Chemical Formula	# Valence e's in Molecule	Lewis Structure	Name of VSEPR Arrangement (Geometry)	Name of Shape (Molecular Geometry)	Bond (Polar or Non–Polar)	Molecule (Polar or Non–Polar)	3 Dimensional Drawing	Resonance (Yes or No)
H_2O						Polar		No
NH_3						Polar		No
CH_4								No
C_2H_4			Around 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_3						Non–Polar		Yes

Molecular Modeling: Bonding & Lewis Structures

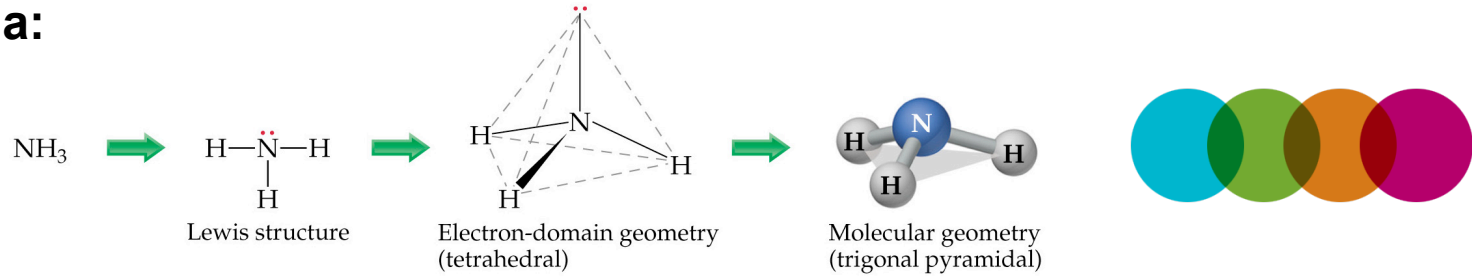
Computational Chemistry: Molecular Modeling Report Form

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:



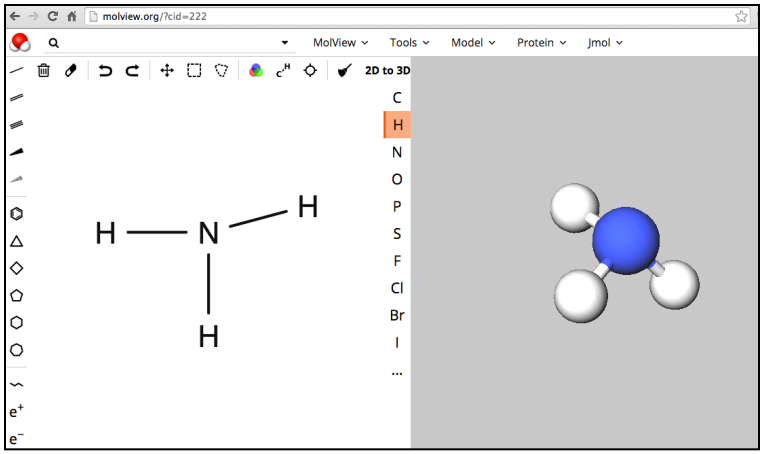
Eg. Ammonia:

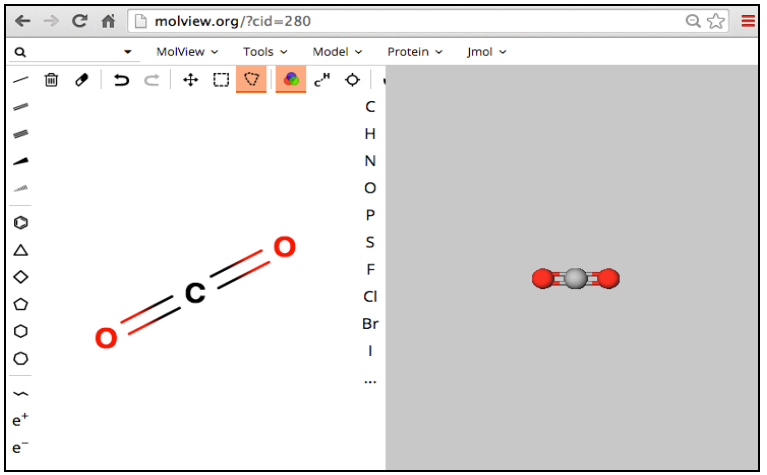


http://molview.org

Molecular Shapes ⟺ Lewis Structures

MolView: Visual On-line Molecular Modeling





Bonding, Lewis Structures, Molecular Modeling:
Computational Experiments

http://molview.org

Molecular Shapes → Lewis Structures

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)
N_2		N N						No
Ammonium $(NH_4)^+$		H H N H H				Polyatomic Ion		No
PBr_3		Br P Br Br				Polar		No
$(NO_2)^-$		O N O				Polyatomic Ion		Yes
$(CO_3)^{2-}$		O C O O				Polyatomic Ion		Yes
CH_2O		O C H H						No

Molecular Modeling: Bonding & Lewis Structures

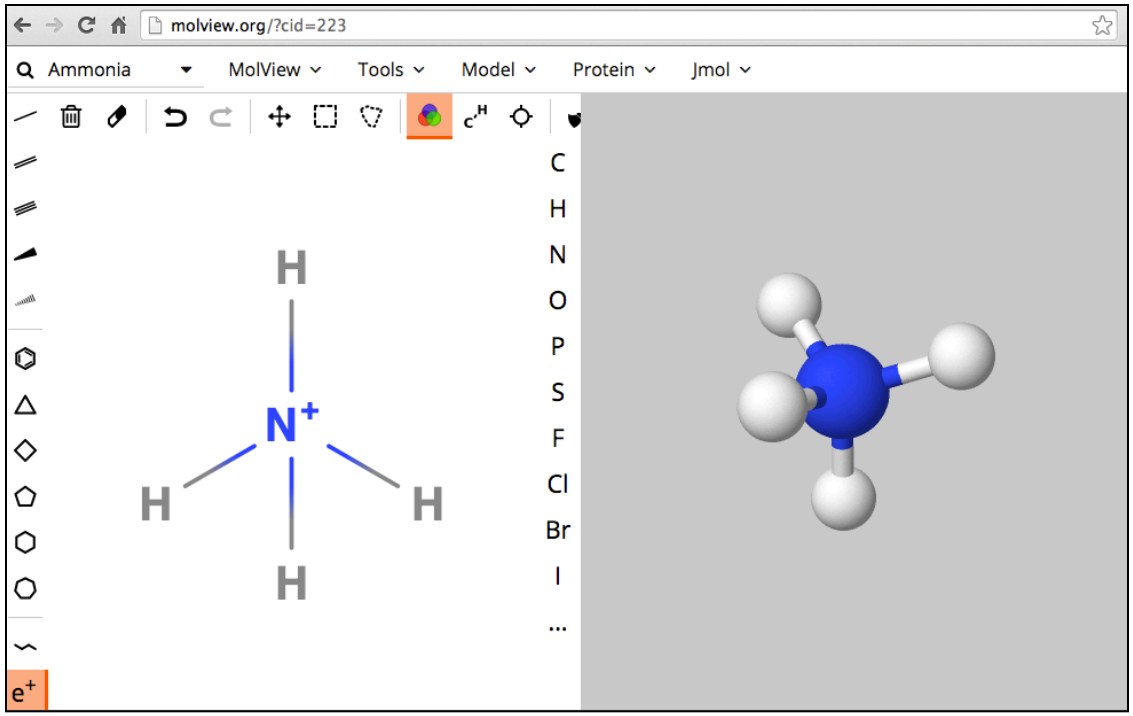
Computational Chemistry: Molecular Modeling Report Form

http://molview.org

Molecular Shapes → Lewis Structures

MolView: Visual On-line Molecular Modeling

Ammonium

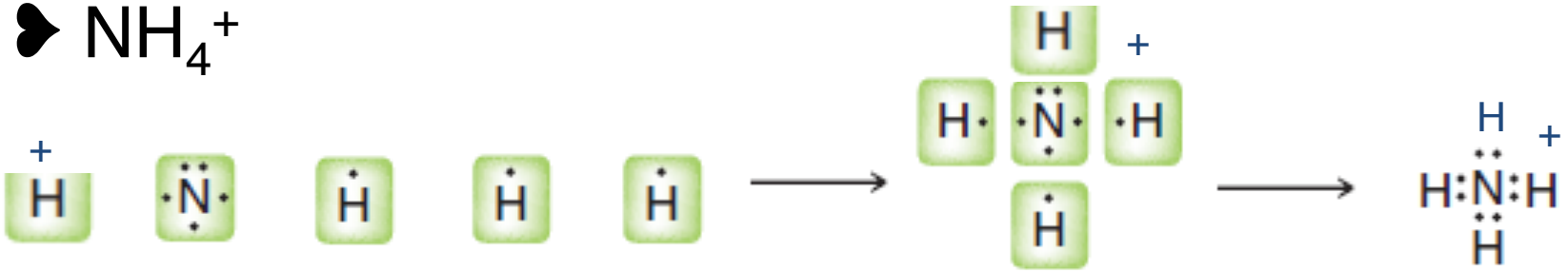


Molecular Modeling: Bonding & Lewis Structures

Computational Chemistry: Molecular Modeling Report Form

Lewis Structures → Molecular Shapes

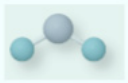
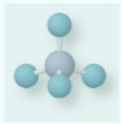
- For simple Lewis structures:
  1. Draw the individual atoms using dots to represent the valence electrons.
  2. Put the atoms together so they share PAIRS of electrons to make complete octets.
- NH_4^+

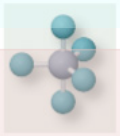


Ammonium

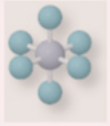
	Orbital (Electronic) Geometry	Molecular Geometry	Bond Angle	# of lone pairs
Important in Organic Compounds	Linear	Linear	180°	0
	Trigonal Planar	Trigonal Planar	120°	0
	Trigonal Planar	Bent	<120°	1
	Tetrahedral	Tetrahedral	109.5°	0
	Tetrahedral	Trigonal Pyramidal	<109.5°	1
	Tetrahedral	Bent	<109.5°	2
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

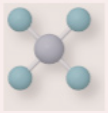


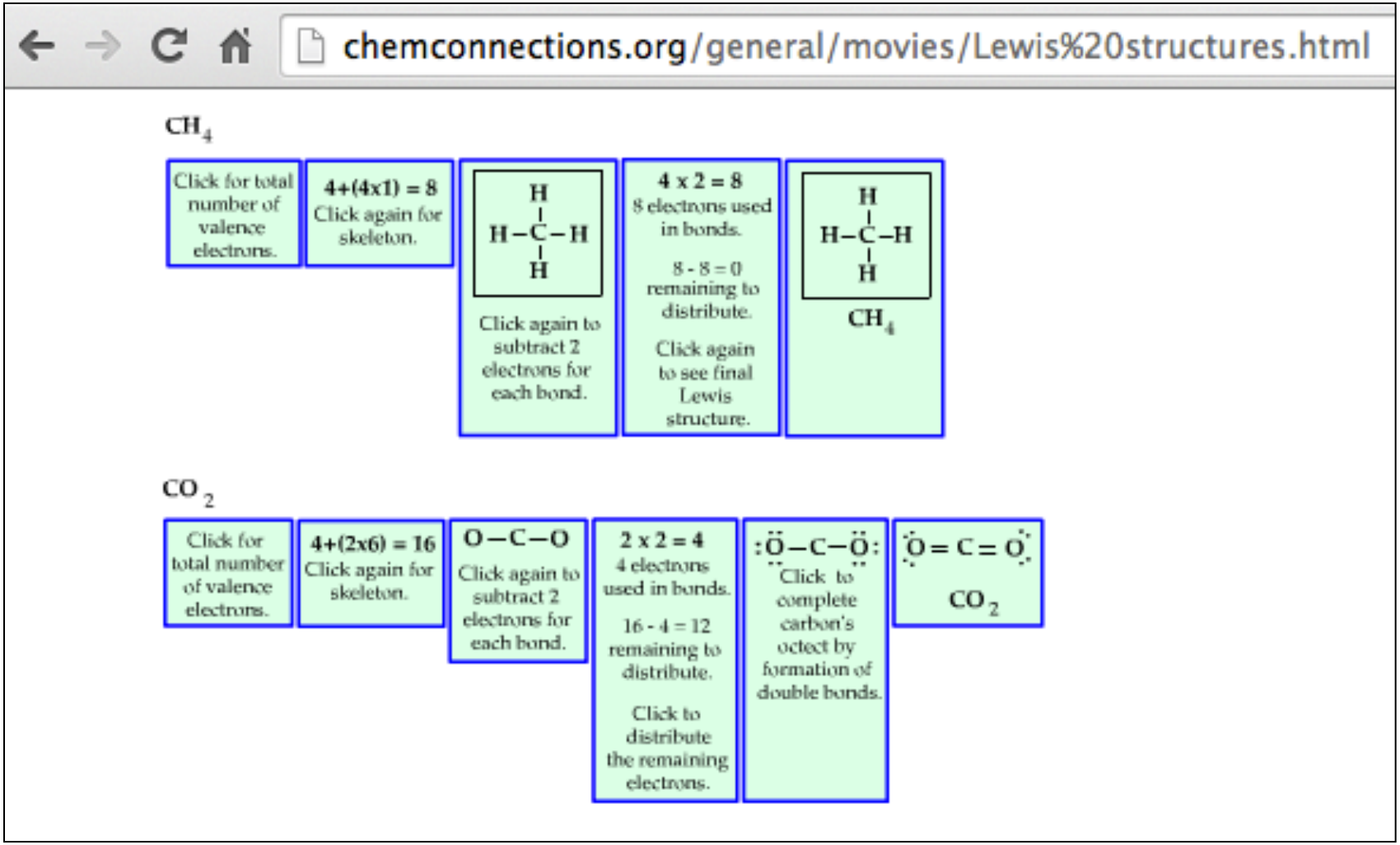









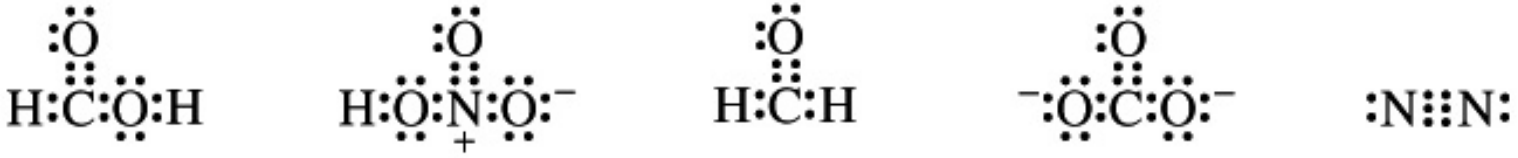
http://chemconnections.org/general/movies/Lewis%20structures.html



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



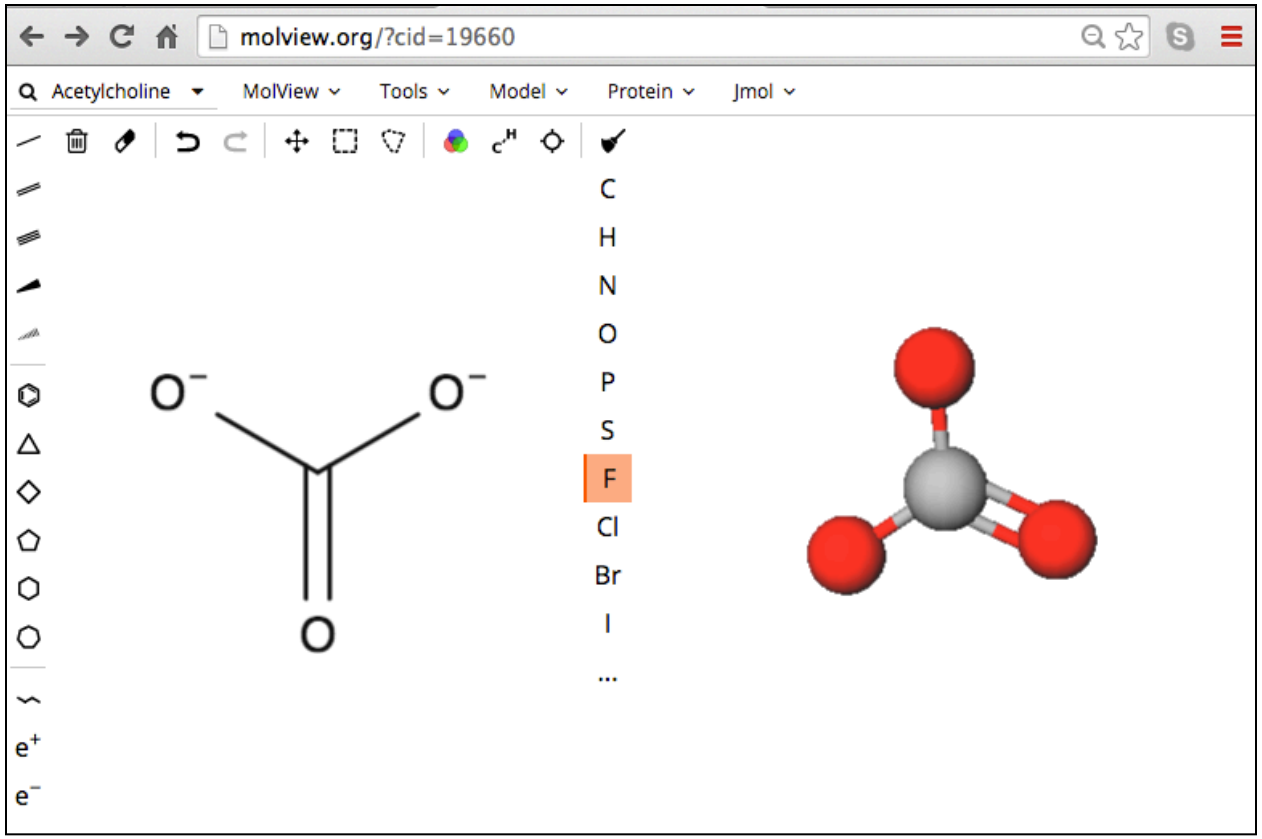
Notice the charges:
In one case they balance, can you name the compound?
In the other they do not.

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

http://molview.org

Molecular Shapes ⟷ Lewis Structures

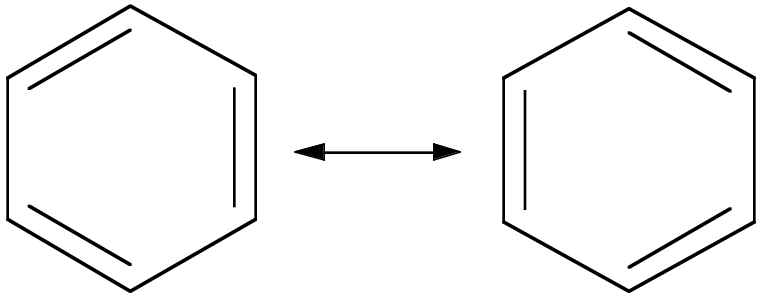
MolView: Polyatomic Ions



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.