

Molecular Modeling Computational Chemistry

<http://molview.org>

Shapes → Lewis Structures

Covalent Bonds:
Lewis Structures, Molecular
Shapes

Dr. Ron Rusay



Except where otherwise noted, content on this site is licensed under a [Creative Commons Attribution 4.0 International license](https://creativecommons.org/licenses/by/4.0/).

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

Shapes of Molecules



What is the Shape of a Molecule?

View the video and complete the Guiding Questions that follow.

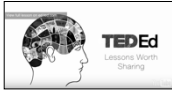
*Required

Name: _____

DATE: _____

View: What is the shape of a molecule?

George Zaidan and Charles Morton

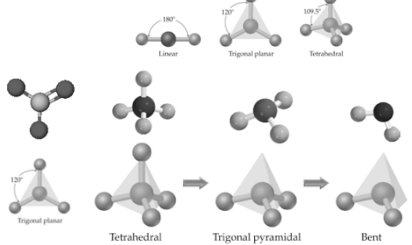


<http://chemconnections.org/general/chem108/Molecular%252520Shapes-Guide.html>

Molecular Shapes

Molecular Models for C, H, N, O

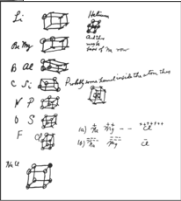
► Fundamental repeating shapes found in every biological and synthetically made organic molecule



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

		1A(1)	2A(2)						
		ns^1	ns^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 •
	3	• Na	• Mg •	• Al •	• Si •	• P •	• S •	• Cl •	• Ar •

• H

• C •

• N •

• O •

Covalent Bond Numbers

(Neutral Atoms!)

one bond

H — F — Cl — Br — I —

two bonds

O —

|

three bonds

— N —

|

four bonds

— C —

|

Linear Trigonal Planar Tetrahedral Trigonal Pyramidal Bent

molecular shape

electronic shape (VSEPR: Electron Domain)

Symbol	Valence electrons	Number of Bonds	Types	Shape	
				electron	molecule
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) Chen H. Dr. Rupp

Name: _____

Molecular Modeling Report Form

These pages replace the Molecular Model Lab pp. 67-101 of the Chemistry 101 Experiments 1st Edition. 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 formulae for a number of compounds. The bonding type is to be determined for these compounds using differences in their respective electronegativity values (order in the is also indicated). The second column is for the electronegativity difference, the double value of the difference in electronegativity between the 2 different atoms in the compound. (SD) = (SD₁ - SD₂). The third column is for the average electronegativity of the two atoms. (SD₁ + SD₂)/2.

Compound	SD ₁ - SD ₂	SD ₁ + SD ₂ 2	Bonding Type
HF	4.0 - 2.1 = 1.9	3.0	polar covalent
HCl			
HBr			
HI			
CuF			
NaF			
CaO			
BaO			
NH ₃			
CH ₄			
CCl ₄			
H ₂ O			
NO			
SO ₂			
H ₂			
O ₂			

<http://molview.org>

Molecular Shapes → Lewis Structures

Report Form - Molecular Models

Chemical Formula	# Valence e ⁻ 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 ₂ O						Polar		No
NH ₃						Polar		No
CH ₄								No
C ₂ H ₆			Around each C	Around each C	C-H C-C	Non-Polar		No
HCl			Around C	Around C	C-H	Polar		No
C ₂ H ₄			Around each C	Around each C	C-H C=C			No
SO ₂						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.

► NH₃, for example:

Eg. Ammonia:

<http://molview.org>

Molecular Shapes ↔ Lewis Structures
MolView: Visual On-line Molecular Modeling

Bonding, Lewis Structures, Molecular Modeling:
Computational Experiments

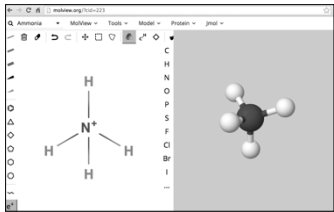
<http://molview.org>

Molecular Shapes → Lewis Structures

Chemical Formula	# Valence e ⁻ 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								No
Ammonium (NH ₄) ⁺						Polystatic ion		No
PBr ₃						Polar		No
(NO ₂) ⁺						Polystatic ion		Yes
(CO ₃) ²⁻						Polystatic ion		Yes
CH ₃ O								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

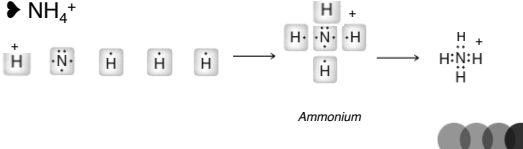
Molecular Modeling: Bonding & Lewis Structures
 Computational Chemistry: Molecular Modeling Report Form

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.

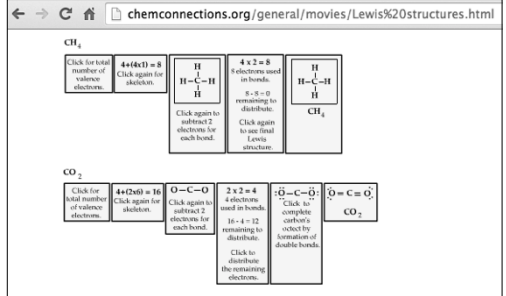
► NH_4^+



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

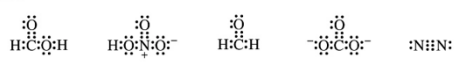
<http://chemconnections.org/general/movies/Lewis%20structures.html>



Covalent Compounds

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

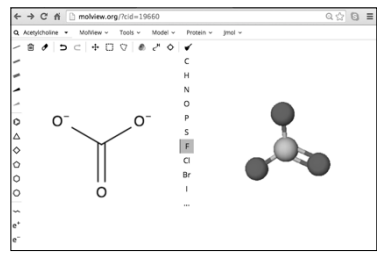
Lewis structures



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?

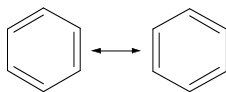
<http://molview.org>
Molecular Shapes ↔ Lewis Structures
 MolView: Polyatomic Ions



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.