Molecular Modeling
Computational Chemistry
Structures ⟷ Shapes

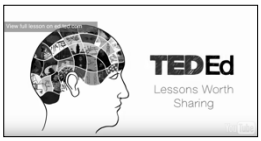
Covalent Bonds:
Lewis Structures, Molecular Shapes

Dr. Ron Rusay

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

Shapes of Molecules

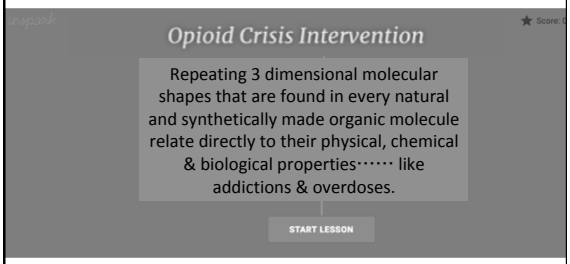
What is the shape of a molecule?
George Zaidan and Charles Morton



Why are the Shapes of Molecules Important?

https://aelp.smartsparrow.com/v/ndmw2ybz/74lytt7u

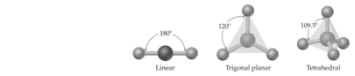
Why are the Shapes of Molecules Important?

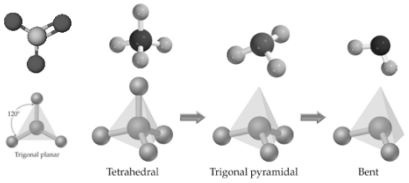


https://aelp.smartsparrow.com/v/ndmw2ybz/74lytt7u

Molecular Shapes
Molecular Models for C, H, N, O

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

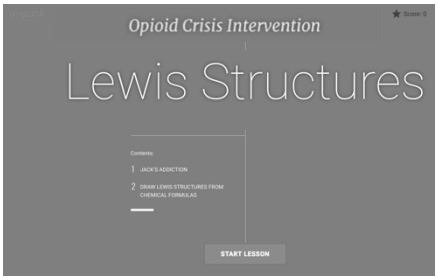




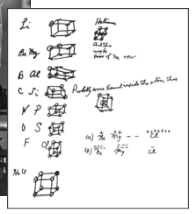
C =black
H = gray
N = blue
O = red

pink = generic atom

https://aelp.smartsparrow.com/v/ndmw2ybz/74lytt7u



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

Covalent Bond Numbers

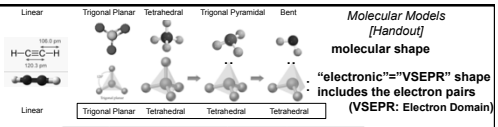
(Neutral Atoms!)

one bond H — F — Cl — Br — I —

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/Lab/Modeling%20molecular%20structures.2020s.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/Lab/Modeling%20molecular%20structures.2020s.pdf

http://molview.org

Lewis Structures ↔ Molecular Shapes

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)
H_2O						Polar
NH_3						Polar
CH_4						
C_2H_4			Around each C	Around each C	C–H C–C	Non–Polar
HCN			Around C	Around C	H–C C–N	Polar
C_2H_2			Around each C	Around each C	C–H C–C	
SO_2						Non–Polar

Molecular Modeling: Bonding & Lewis Structures
Computational Chemistry: Molecular Modeling Form
http://chemconnections.org/general/chem108/Molecular%20Modeling%20form%202020.pdf

http://molview.org

Lewis Structures ↔ Molecular Shapes

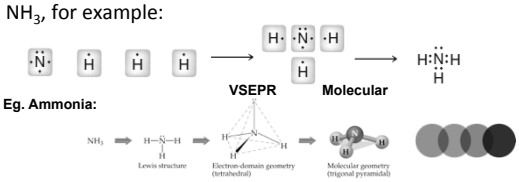
Name?
Ammonia

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)
H_2O						Polar
NH_3	8					Polar
CH_4						
C_2H_4			Around each C	Around each C	C-H C-C	Non-Polar
HCN			Around C	Around C	H-C C-N	Polar
C_2H_2			Around each C	Around each C	C-H C-C	
SO_3						Non-Polar

Molecular Modeling: Bonding & Lewis Structures
Computational Chemistry: Molecular Modeling Form
http://chemconnections.org/general/chem108/Molecular%20Modeling%20form%202020.pdf

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:



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Lewis Structures ↔ Molecular Shapes

Name?
Ammonia

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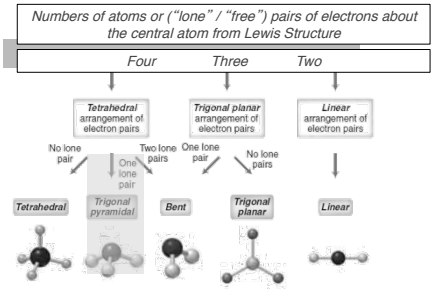
Molecular Geometry – Lewis Structure



unbonded e⁻ = "free" lone pairs x 2

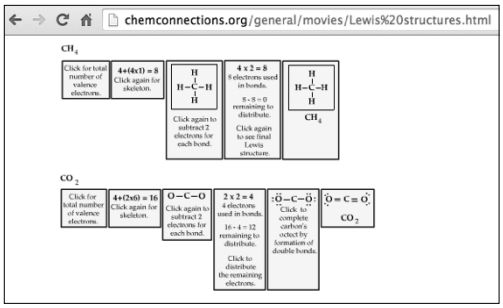
Lewis Structures / Covalent Compounds

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

Lewis structures

Total e's	18	24	12	24	10
bonded	10	10	8	8	6
un-bonded	8	14	4	16	4

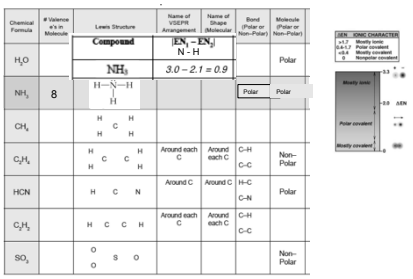
http://chemconnections.org/general/movies/Lewis%20structures.html



http://molview.org

Lewis Structures ↔ Molecular Shapes

Name?
Ammonia



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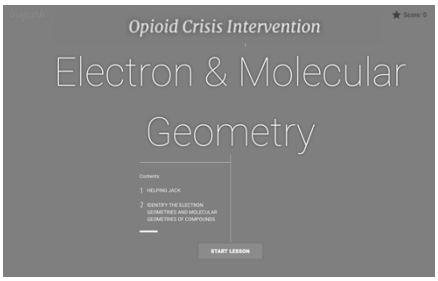
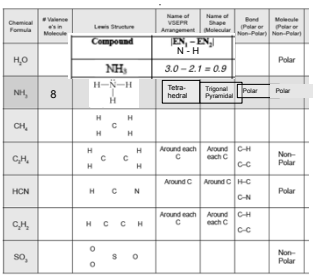


	VSEPR (Electronic) Geometry	Molecular Geometry	Bond Angle	# of lone pairs
Important in Organic Compounds	Linear	Linear	180°	0
	Trigonal Planar	Trigonal Planar	120°	0
	Trigonal Planar	Bent	<120°	1
	Tetrahedral	Tetrahedral	109.5°	0
	Tetrahedral	Trigonal Pyramidal	<109.5°	1
	Tetrahedral	Bent	<109.5°	2
See 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://molview.org

Lewis Structures ↔ Molecular Shapes

Name?
Ammonia



Polar Bond
N - H

polar molecule overall

Molecular Modeling: Bonding & Lewis Structures
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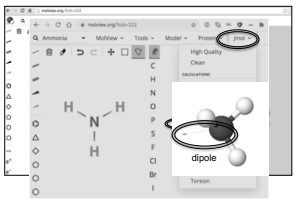
http://molview.org

Molecular Shapes ↔ Lewis Structures

MolView: Visual On-line Molecular Modeling



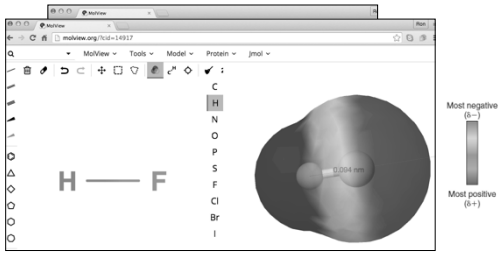
polar molecule overall

Bonding, Lewis Structures, Molecular Modeling: Computational Experiments

http://chemconnections.org/general/chem108/Molecular%20Modeling%20form%202020.pdf

Polarity & Modeling

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



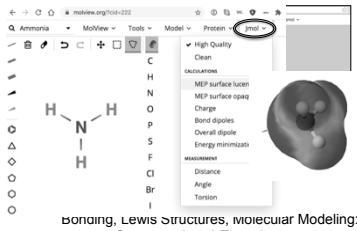
Color coded electron density distribution: red-highest, blue lowest, green balanced

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

http://molview.org

Molecular Shapes ⟷ Lewis Structures

MolView: Visual On-line Molecular Modeling



Bonding, Lewis Structures, Molecular Modeling: Computational Experiments

polar molecule overall

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http://molview.org

Lewis Structures ↔ Molecular Shapes

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)
H_2O	8		tetrahedral	bent	polar	Polar
NH_3	8		tetrahedral	trigonal pyramidal	polar	Polar
CH_4	8		tetrahedral	tetrahedral	non-polar	non-polar
C_2H_4	12		Around each C Trig Planar	Around each C Trig Planar	C–H Linear C–C Linear	Non-Polar
HCN	10	H – C ≡ N:	Around C Linear	Around C Linear	H–C Linear C–N Linear	Polar
C_2H_2	10	H – C ≡ C – H	Around each C Linear	Around each C Linear	C–H Linear C–C Linear	non-polar
SO_3	24		trigonal planar	trig. planar	polar	Non-Polar

Name?

Ammonia

ethylene

Mole res

Comp form

http://chemconnections.org/general/chem108/Molecular%20Modeling%20form%202020.pdf

http://molview.org

Lewis Structures ↔ Molecular Shapes

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)
CBr_4		Br, C, Br, Br, Br				
CO_2		O C O				
H_2S		S, H, H				
NF_3		F, N, F, F				
SO_2		S, O, O				Polar
CH_3OH		H, H C O H, H	Around C Around O	Around C Around O	C–H C–O O–H	Polar
$(NO_3)^-$		O, N, O, O				Polyatomic Ion

http://chemconnections.org/general/chem108/Molecular%20Modeling%20form%202020.pdf

http://molview.org

Lewis Structures ↔ Molecular Shapes

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)
CBr_4	32		tetrahedral	tetrahedral	polar	non-polar
CO_2	16	O = C = O	linear	linear	polar	non-polar
H_2S	8		tetrahedral	bent	polar	polar
NF_3	26		tetrahedral	trig. pyramidal	polar	polar
SO_2	18		trigonal planar	bent	polar	Polar
CH_3OH	14		Around C Tetrhedral Around O Tetrhedral	Around C Tetrhedral Around O Bent	C–H nonpolar C–O polar O–H polar	Polar
$(NO_3)^-$	24		trigonal planar	trigonal planar	polar	Polyatomic Ion

http://chemconnections.org/general/chem108/Molecular%20Modeling%20form%202020.pdf

http://molview.org

Lewis Structures ↔ Molecular Shapes

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)
N_2		N N				
$(NH_4)^+$		H, N, H, H, H				Polyatomic Ion
PBr_3		Br, P, Br, Br				Polar
$(NO_3)^-$		O, N, O, O				Polyatomic Ion
$(CO_3)^{2-}$		O, C, O, O				Polyatomic Ion
CH_2O		O, C, H, H				

http://chemconnections.org/general/chem108/Molecular%20Modeling%20form%202020.pdf

http://molview.org

Lewis Structures ↔ Molecular Shapes

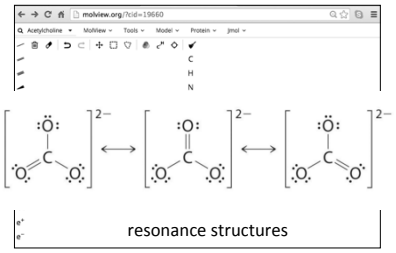
Chemical Formula	# Valence e's in Molecule	Lewis Structure	Name of VSEPR Arrangement (Geometry)	Name of Shape (Molecular Geometry)	Bond (Polar or Non-Polar)	Molecule (Polar or Non-Polar)
N_2	10	:N ≡ N:	linear	linear	non-polar	non-polar
$(NH_4)^+$	9		tetrahedral	tetrahedral	polar	Polyatomic Ion
PBr_3	26		tetrahedral	trigonal pyramidal	polar	Polar
$(NO_3)^-$	18		trigonal planar	bent	polar	Polyatomic Ion
$(CO_3)^{2-}$	24		trigonal planar	trigonal planar	polar	Polyatomic Ion
CH_2O	12		trigonal planar	trigonal planar	polar	polar

http://chemconnections.org/general/chem108/Molecular%20Modeling%20form%202020.pdf

http://molview.org

Resonance Models & Lewis Structures

MolView: Carbonate Polyatomic Ion

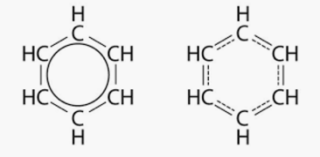


Bonding, Lewis Structures, Molecular Modeling:

http://chemconnections.org/general/chem108/Molecular%20Modeling%20form%202020.pdf

Resonance

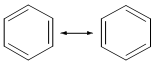
- Occurs when more than one valid Lewis structure can be written for a particular mo , double or t



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

Question

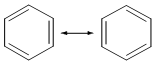
Two resonance structures of benzene, a human carcinogen, with C-C & C=C bonds are shown below. Which statement is incorrect?



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?



A. The double headed arrow indicates that the 2 resonance structures are rapidly interchanging.
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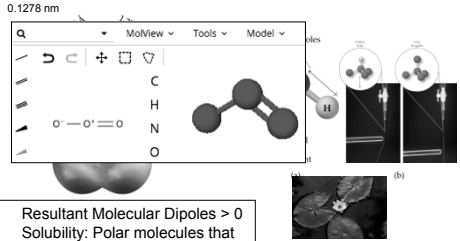
D. The actual bond lengths in benzene are not equal to either single or double bonds.

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

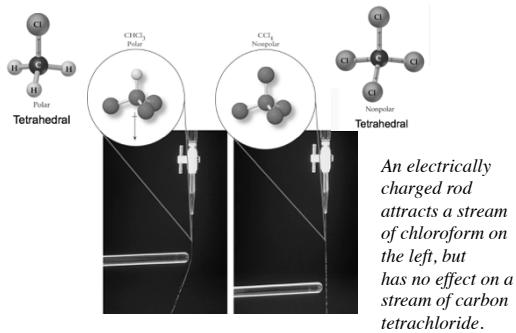
Polarity & Physical Properties

Ozone, Water, & Batteries



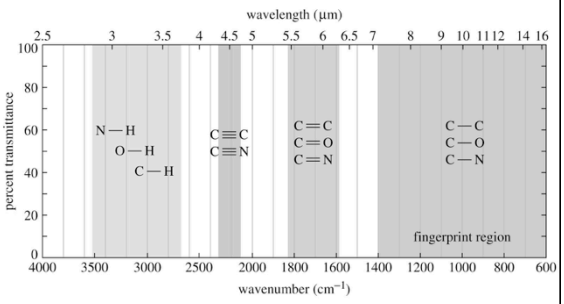
- Resultant Molecular Dipoles > 0
- Solubility: Polar molecules that dissolve or are dissolved in like molecules

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



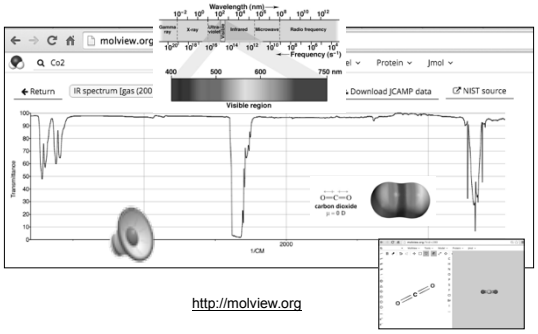
An electrically charged rod attracts a stream of chloroform on the left, but has no effect on a stream of carbon tetrachloride.

Infrared- Bond Absorbances



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

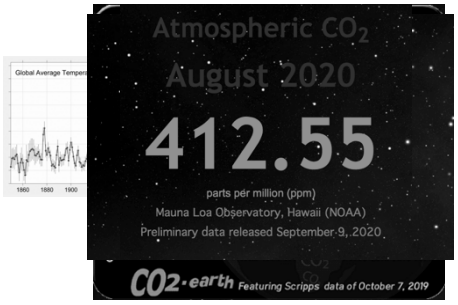
Infrared- Bond Absorbances



http://molview.org

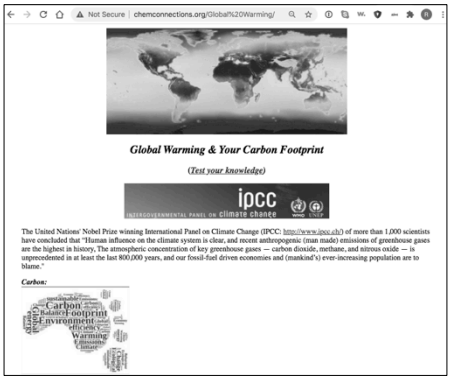
https://www.youtube.com/watch?v=W5gimZlFY6I

Infrared- Bond Absorbances



https://www.co2.earth/

http://chemconnections.org/Global%20Warming/



https://www.youtube.com/watch?v=ypbb9Zi5Tao&list=PLE7B4FAD08F1EBCE2