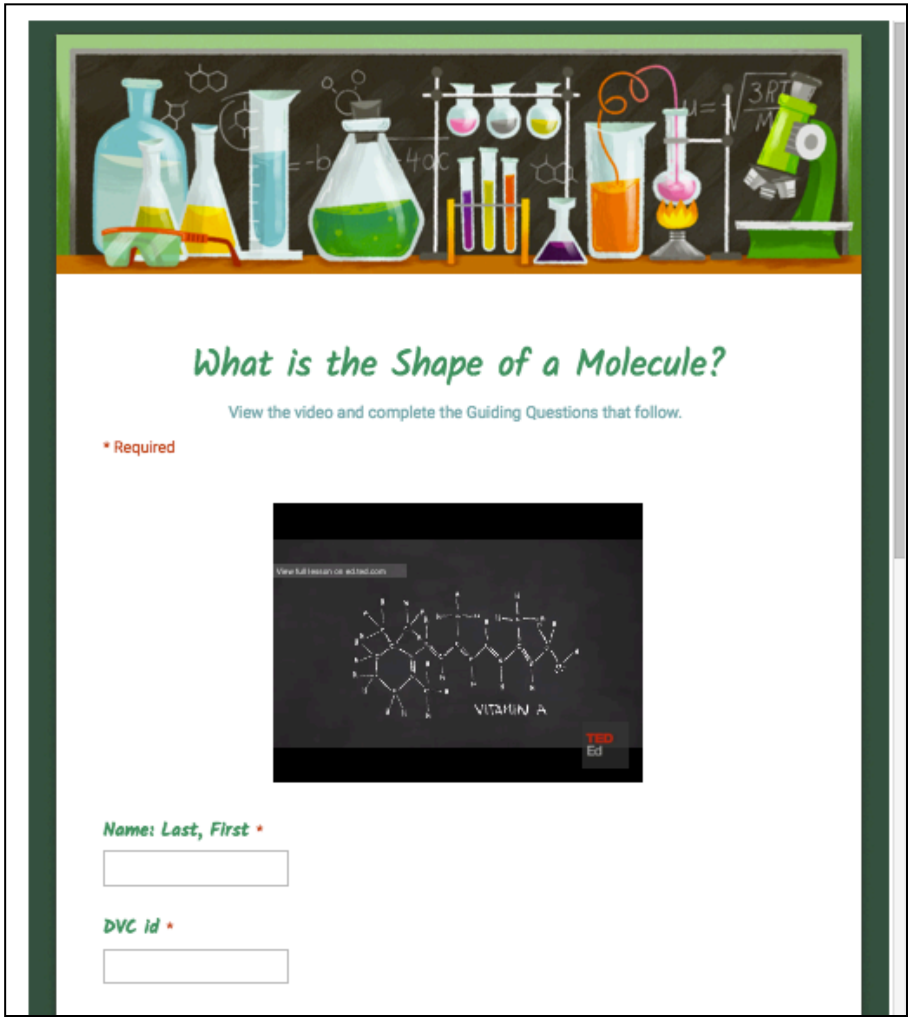
Molecular Modeling
Computational Chemistry

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?

View the video and complete the Guiding Questions that follow.

* Required

Name: Last, First *

DVC id *

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

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

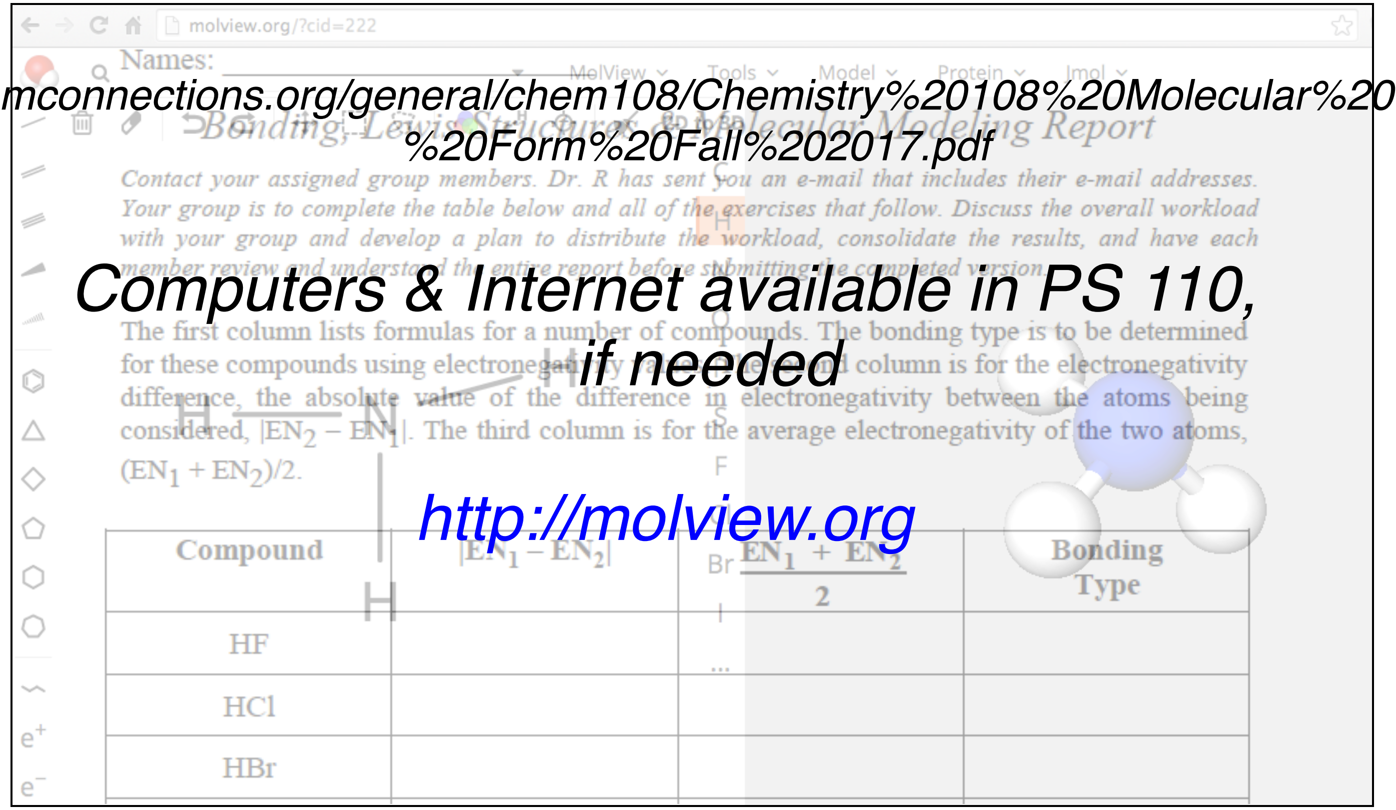
Guiding Questions

Molecular Modeling

(Individual or Collaborative)

Report Form (Replacement pages for Molecular Model Lab pp. 97-103)

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



Names: ____________________

Bonding, Lewis Structures, & Molecular Modeling Report

Contact your assigned group members. Dr. R has sent you an e-mail that includes their e-mail addresses. Your group is to complete the table below and all of the exercises that follow. Discuss the overall workload with your group and develop a plan to distribute the workload, consolidate the results, and have each member review and understand the entire report before submitting the completed version.

The first column lists formulas for a number of compounds. The bonding type is to be determined for these compounds using electronegativity values. The second column is for the electronegativity difference, the absolute value of the difference in electronegativity between the atoms being considered, $|EN_2 - EN_1|$. The third column is for the average electronegativity of the two atoms, $(EN_1 + EN_2)/2$.

Compound	$\|EN_1 - EN_2\|$	$\frac{EN_1 + EN_2}{2}$	Bonding Type
HF			
HCl			
HBr			

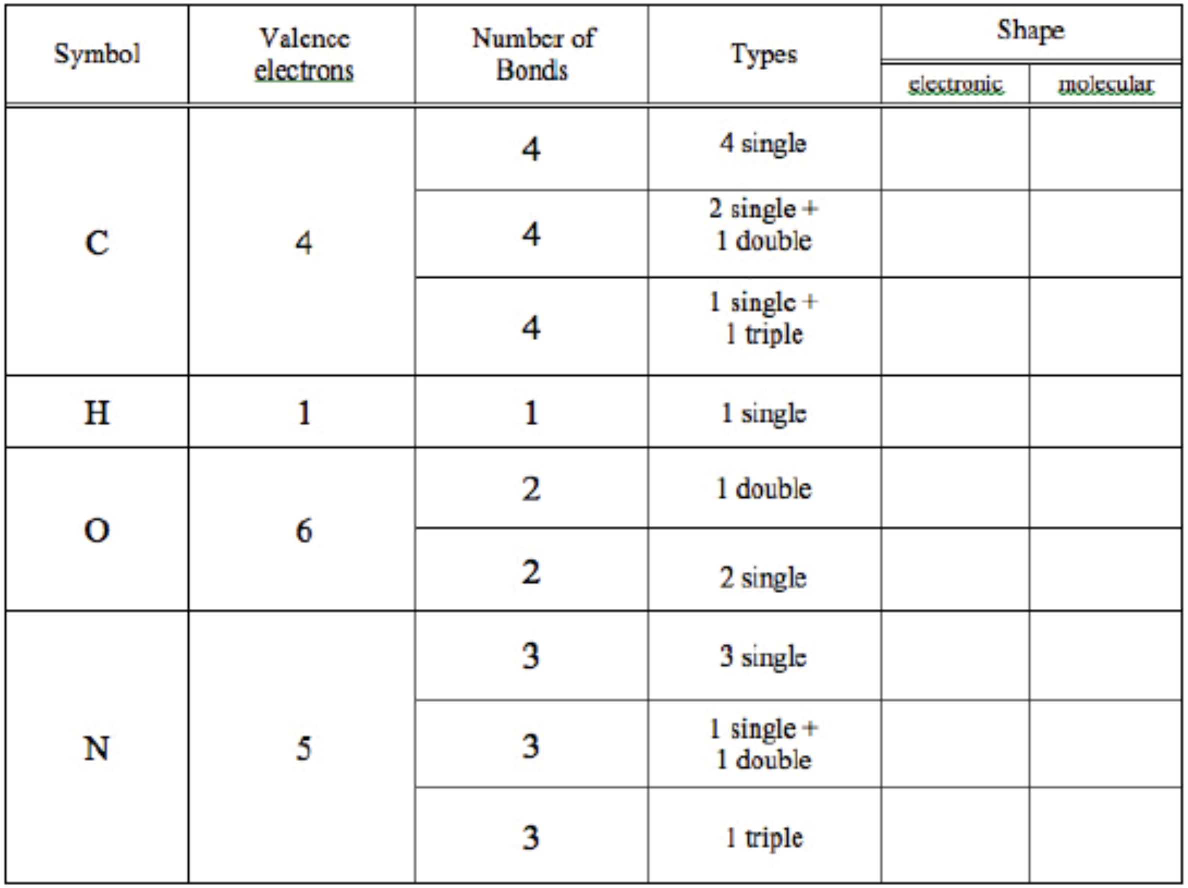
Computers & Internet available in PS 110, *if needed*

http://molview.org

Turn-in individually or one per group

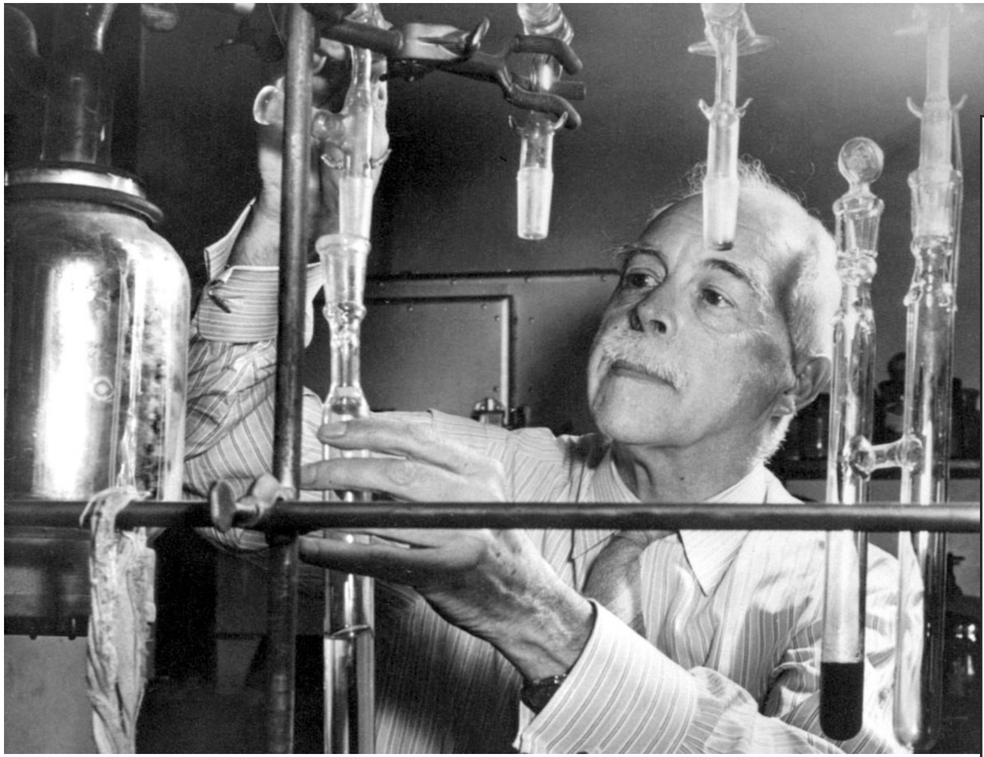
Consult Calendar for Due Date

Important Bond Numbers



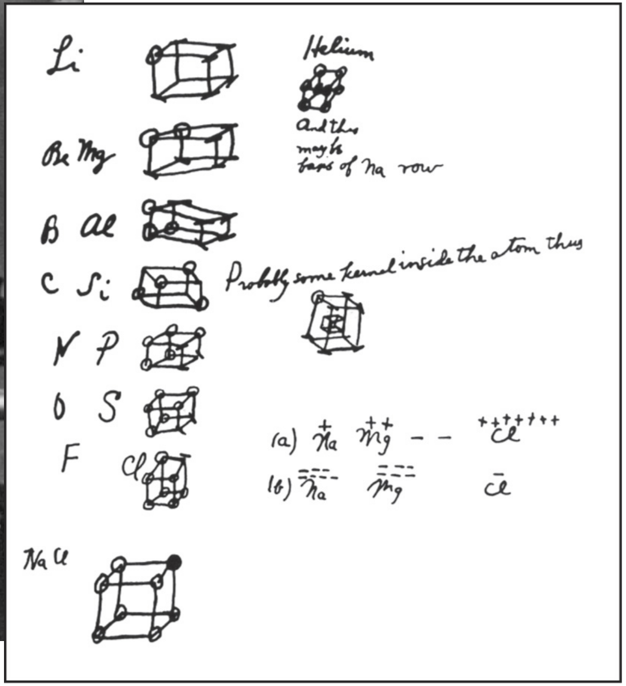
Symbol	Valence electrons	Number of Bonds	Types	Shape	
				electronic	molecular
C	4	4	4 single		
		4	2 single + 1 double		
		4	1 single + 1 triple		
H	1	1	1 single		
O	6	2	1 double		
		2	2 single		
N	5	3	3 single		
		3	1 single + 1 double		
		3	1 triple		

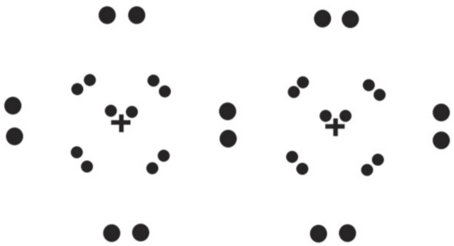
Professor Gilbert Newton Lewis (circa 1940)



G.N. Lewis

Photo Bancroft Library, University of California/LBNL Image Library

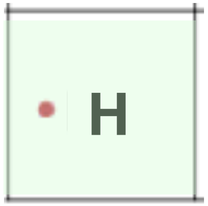




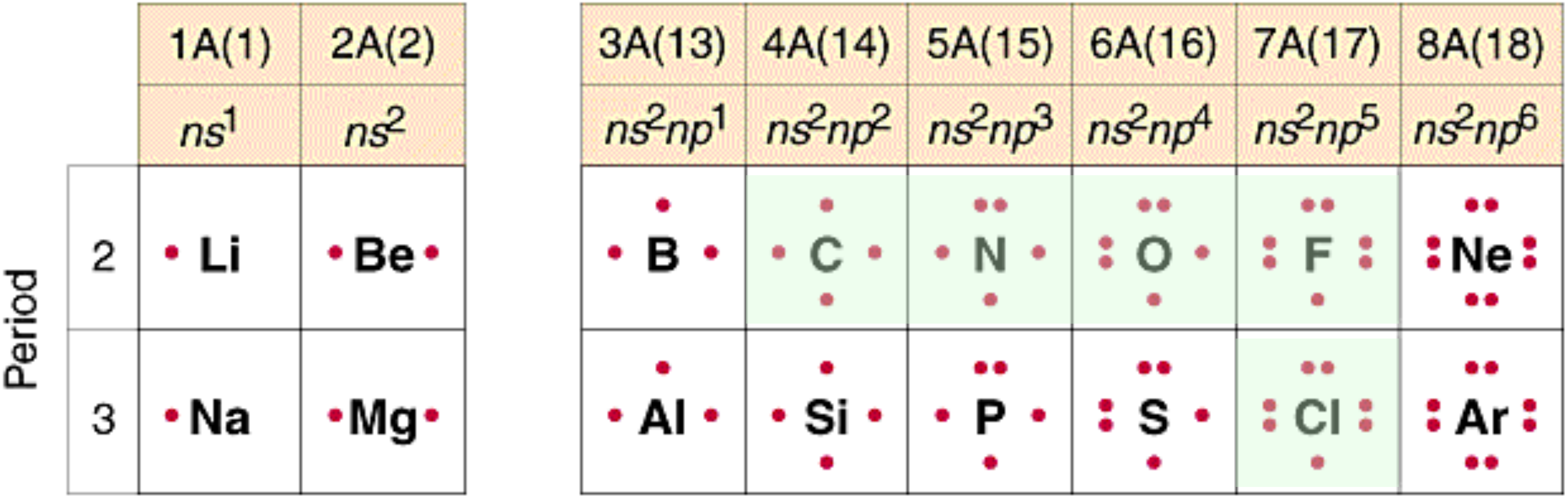
Notes from Lewis's notebook and his "Lewis" structure.

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

Lewis Electron-Dot Drawings



Covalent Bonding-Valence Electrons
Periods 2 & 3

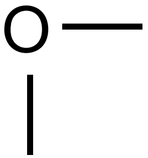


Important Bond Numbers

one bond

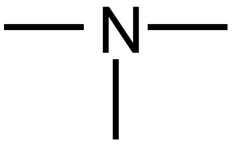
H — F — Cl— Br— I—

two bonds



2 single or 1 double

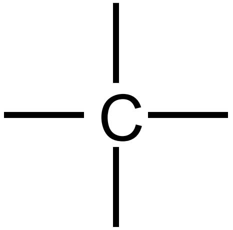
three bonds



3 single or
1 single + 1 double or
1 triple

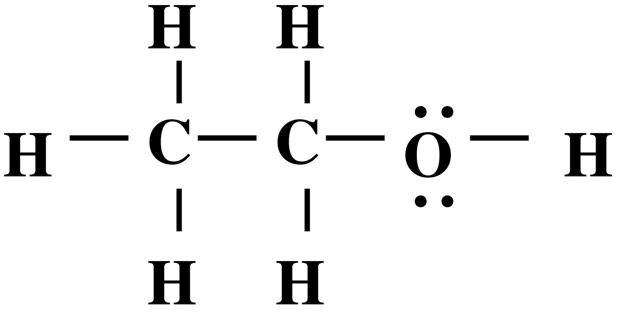
four bonds

4 single or
2 single + 1 double or
1 single + 1 triple or
2 double



Lewis Structures

— *equals 1 pair of e^-s*



Ethyl Alcohol (Ethanol)

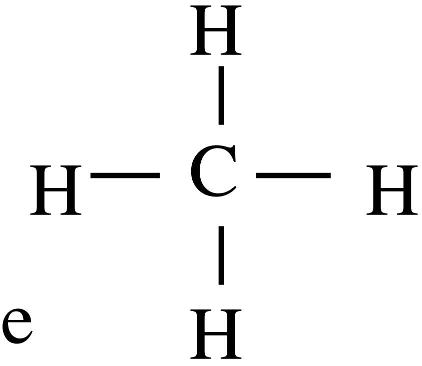
CH_3CH_2OH

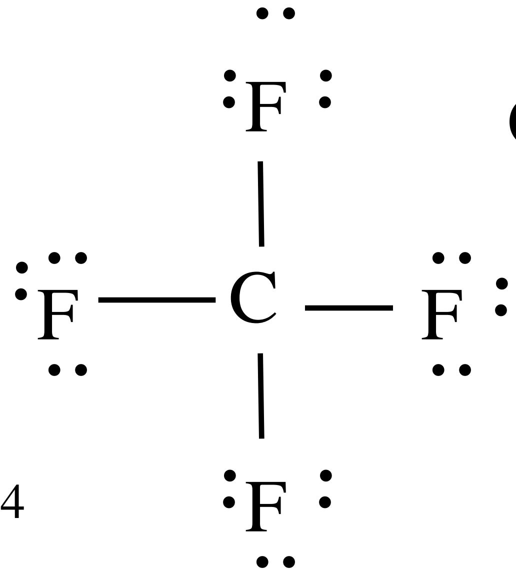
C_2H_5OH

C_2H_6O

CH_4

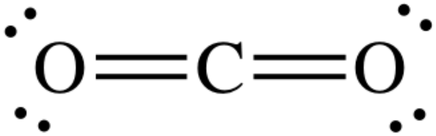
Methane



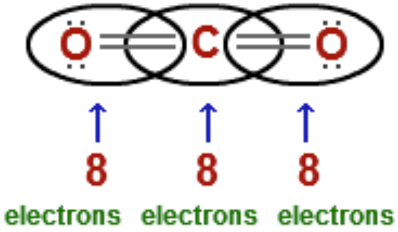


CF_4

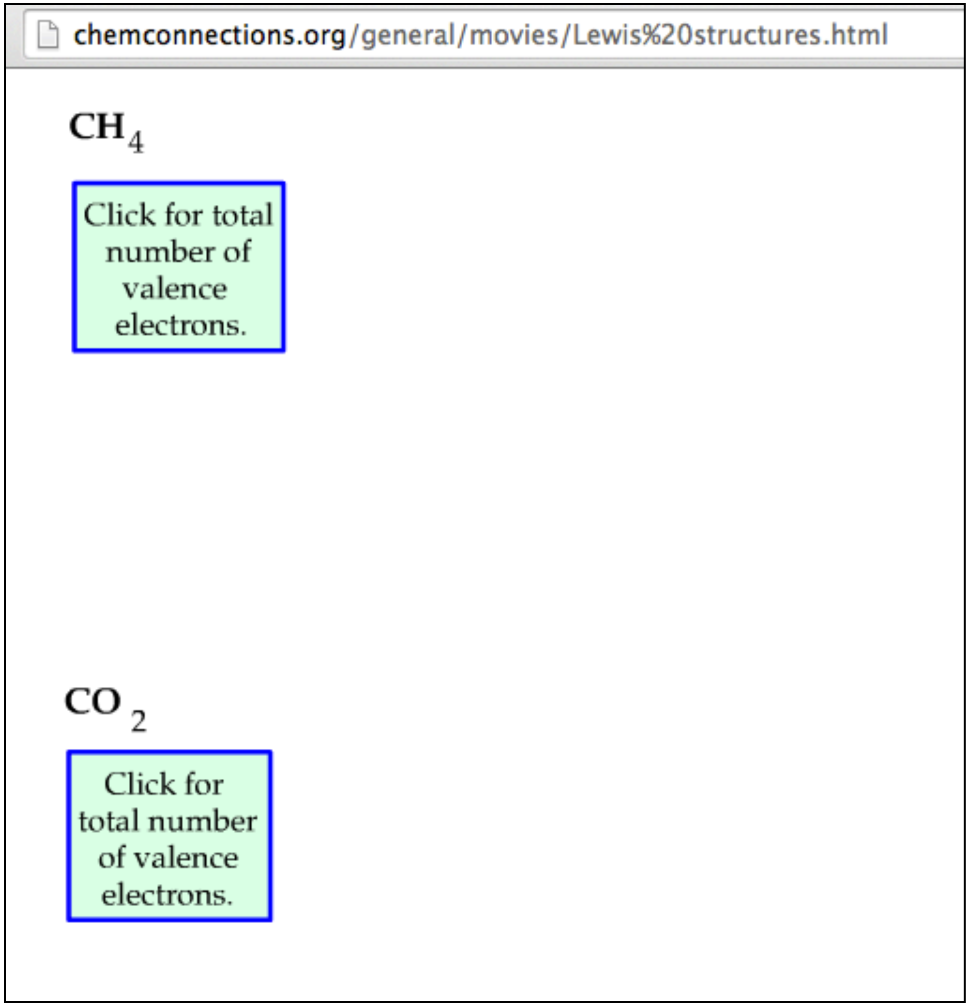
Carbon Tetrafluoride



Carbon dioxide



Note the carbon "double bond"; equals 2 pairs of e^-s *http://chemconnections.org/general/movies/Lewis%20structures.html*



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

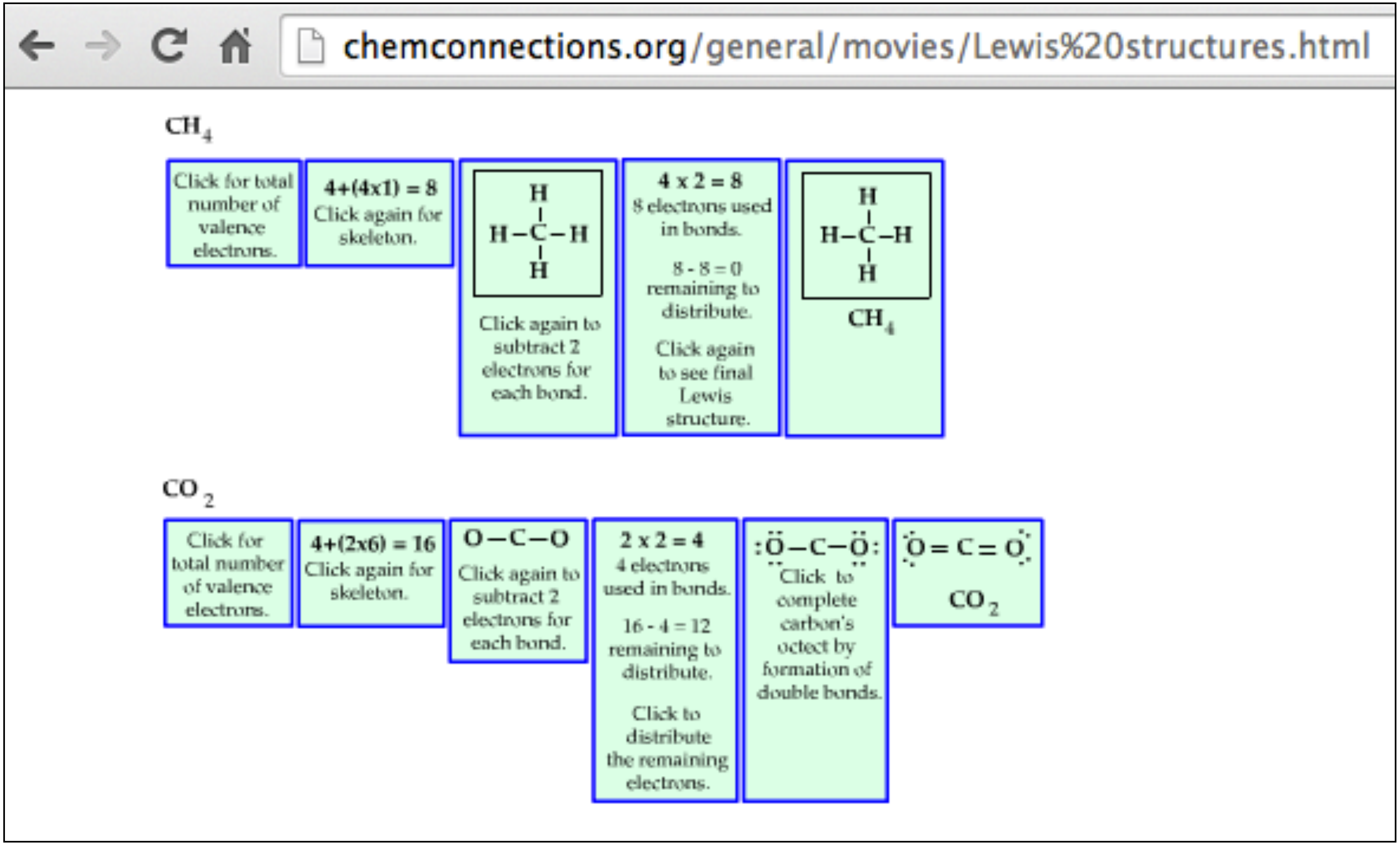
CH_4

Click for total number of valence electrons.

CO_2

Click for total number of valence electrons.

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



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

CH_4

Click for total number of valence electrons.

4+(4x1) = 8
Click again for skeleton.

H
|
H–C–H
|
H

Click again to subtract 2 electrons for each bond.

4 x 2 = 8
8 electrons used in bonds.

8 - 8 = 0
remaining to distribute.

Click again to see final Lewis structure.

H
|
H–C–H
|
H

CH_4

CO_2

Click for total number of valence electrons.

4+(2x6) = 16
Click again for skeleton.

O–C–O

Click again to subtract 2 electrons for each bond.

2 x 2 = 4
4 electrons used in bonds.

16 - 4 = 12
remaining to distribute.

Click to distribute the remaining electrons.

:Ö–C–Ö:

Click to complete carbon's octect by formation of double bonds.

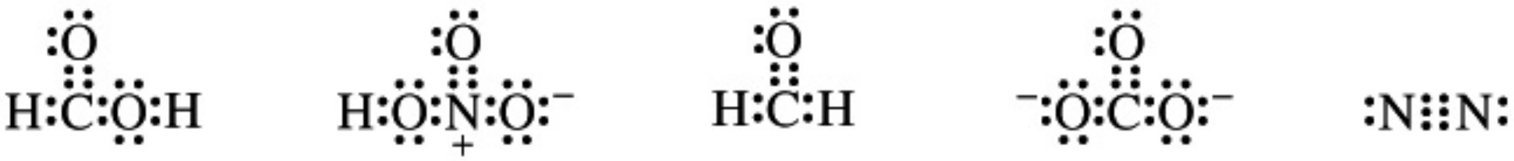
O=C=O

CO_2

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



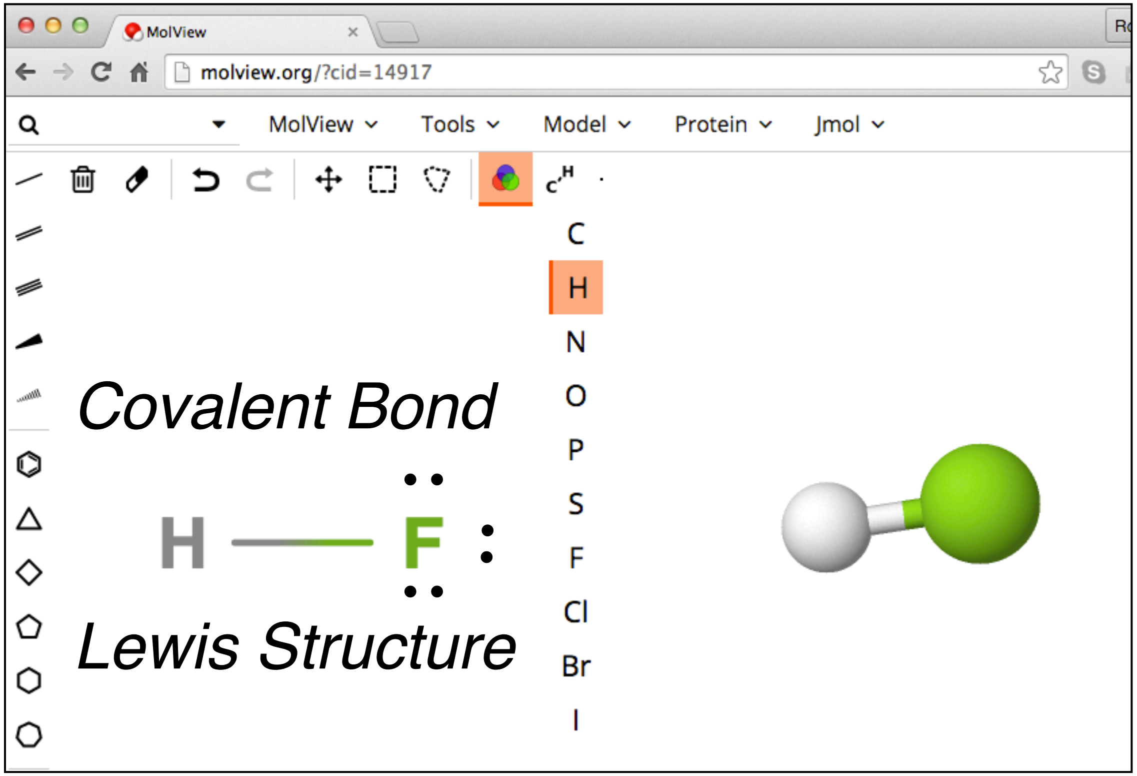
Notice the charges:
In one case they balance, can you name the compound?
In the other they do not.

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

Computational Chemistry

Covalent Bonding

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



Close opening screen; caffeine appears.

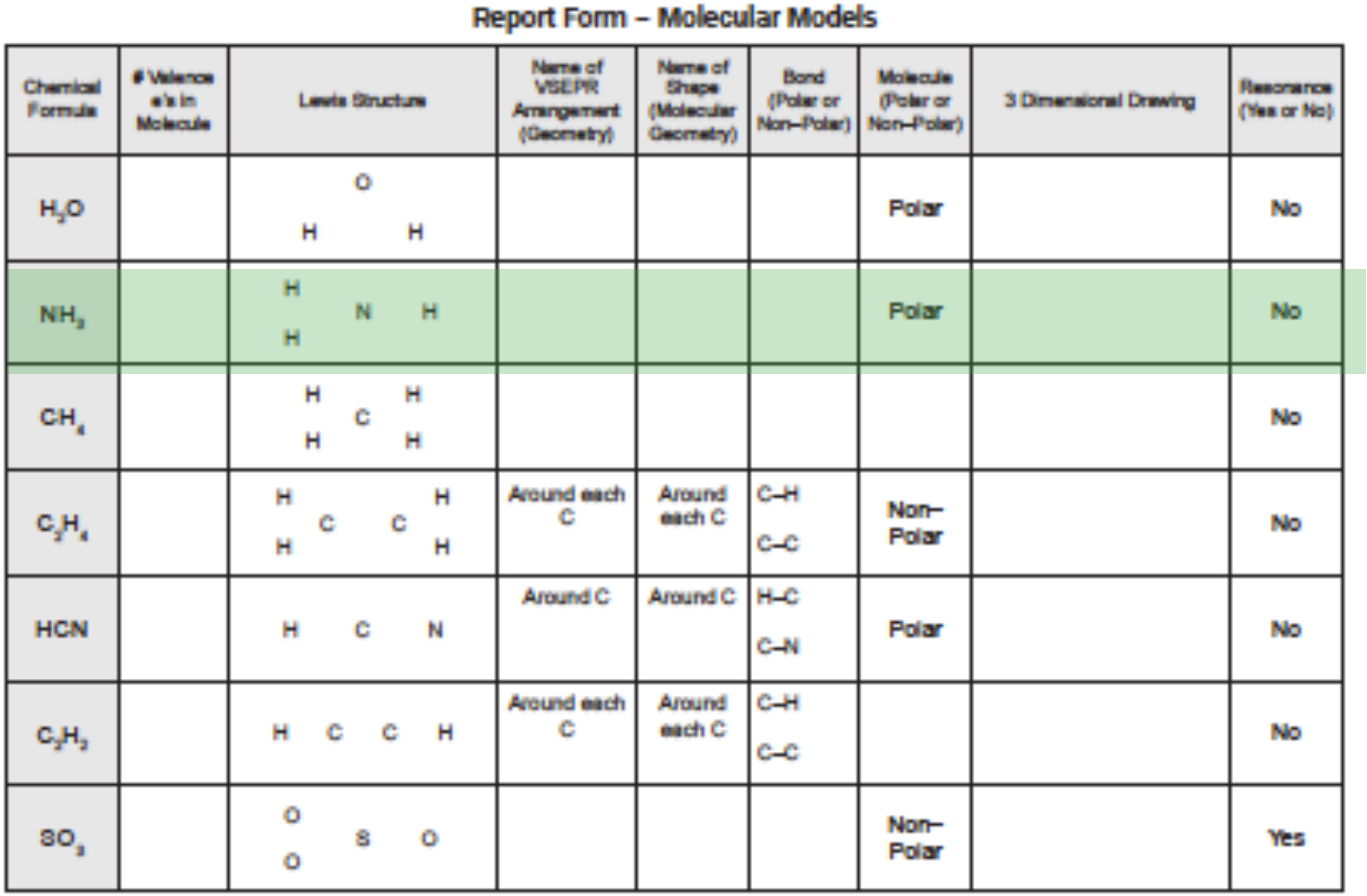
Click trash; now build hydrogen fluoride

http://molview.org

http://molview.org

Molecular Shapes → Lewis Structures

Ammonia



Report Form – Molecular Models

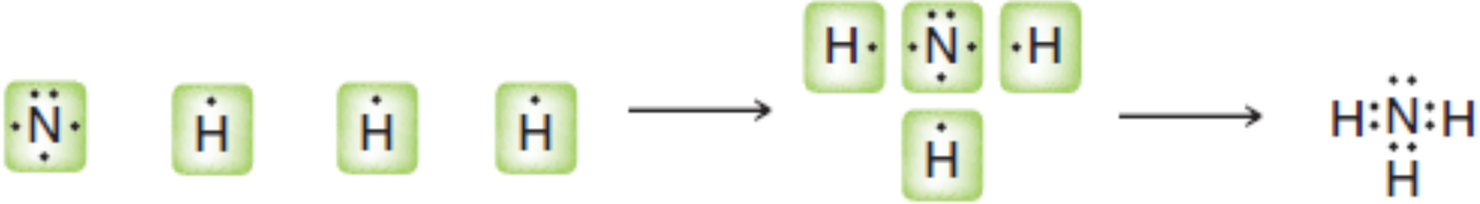
Chemical Formula	# Valence e's in Molecule	Lewis Structure	Name of VSEPR Arrangement (Geometry)	Name of Shape (Molecular Geometry)	Bond (Polar or Non–Polar)	Molecule (Polar or Non–Polar)	3 Dimensional Drawing	Resonance (Yes or No)
H_2O		O H H				Polar		No
NH_3		H N H H				Polar		No
CH_4		H H C H H		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

Molecular Modeling: Bonding & Lewis Structures

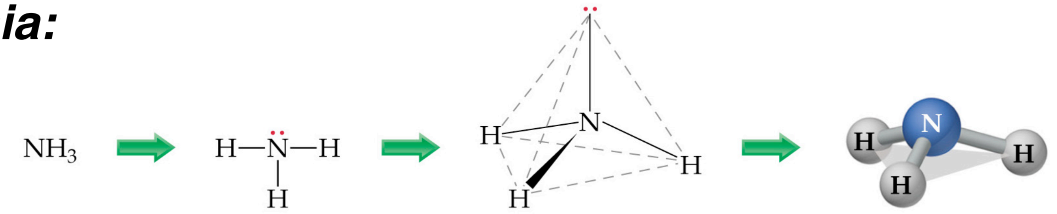
Computational Chemistry: Molecular Modeling Report Form

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:



Lewis structure

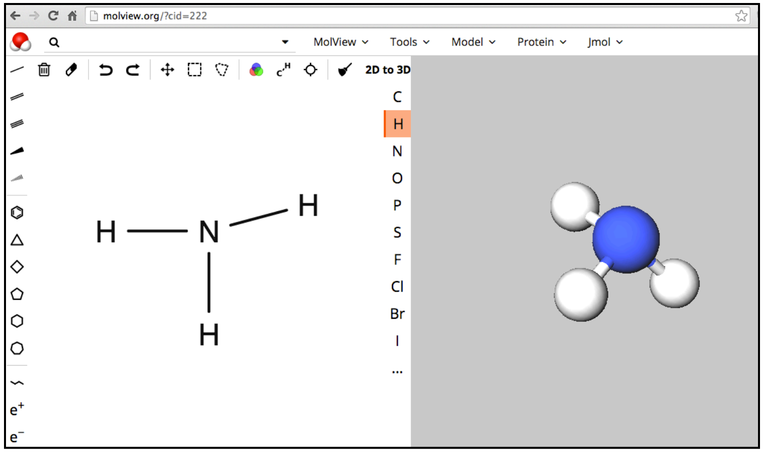
Electron-domain geometry (tetrahedral)

Molecular geometry (trigonal pyramidal)

http://molview.org

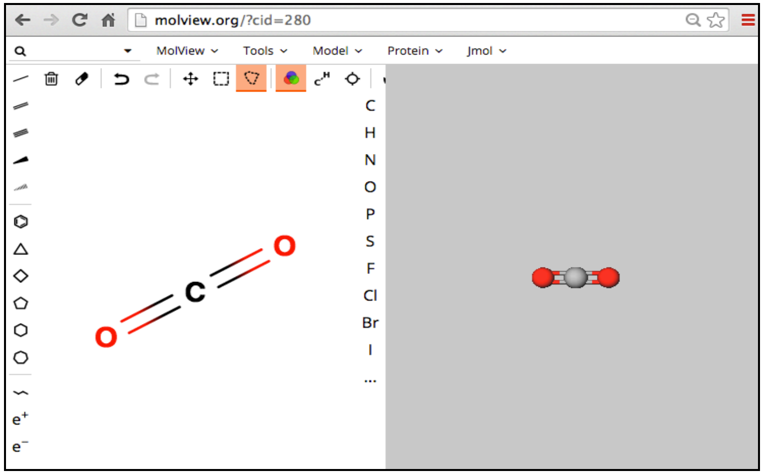
Molecular Shapes ⟷ Lewis Structures

MolView: Visual On-line Molecular Modeling



build ammonia

build carbon dioxide

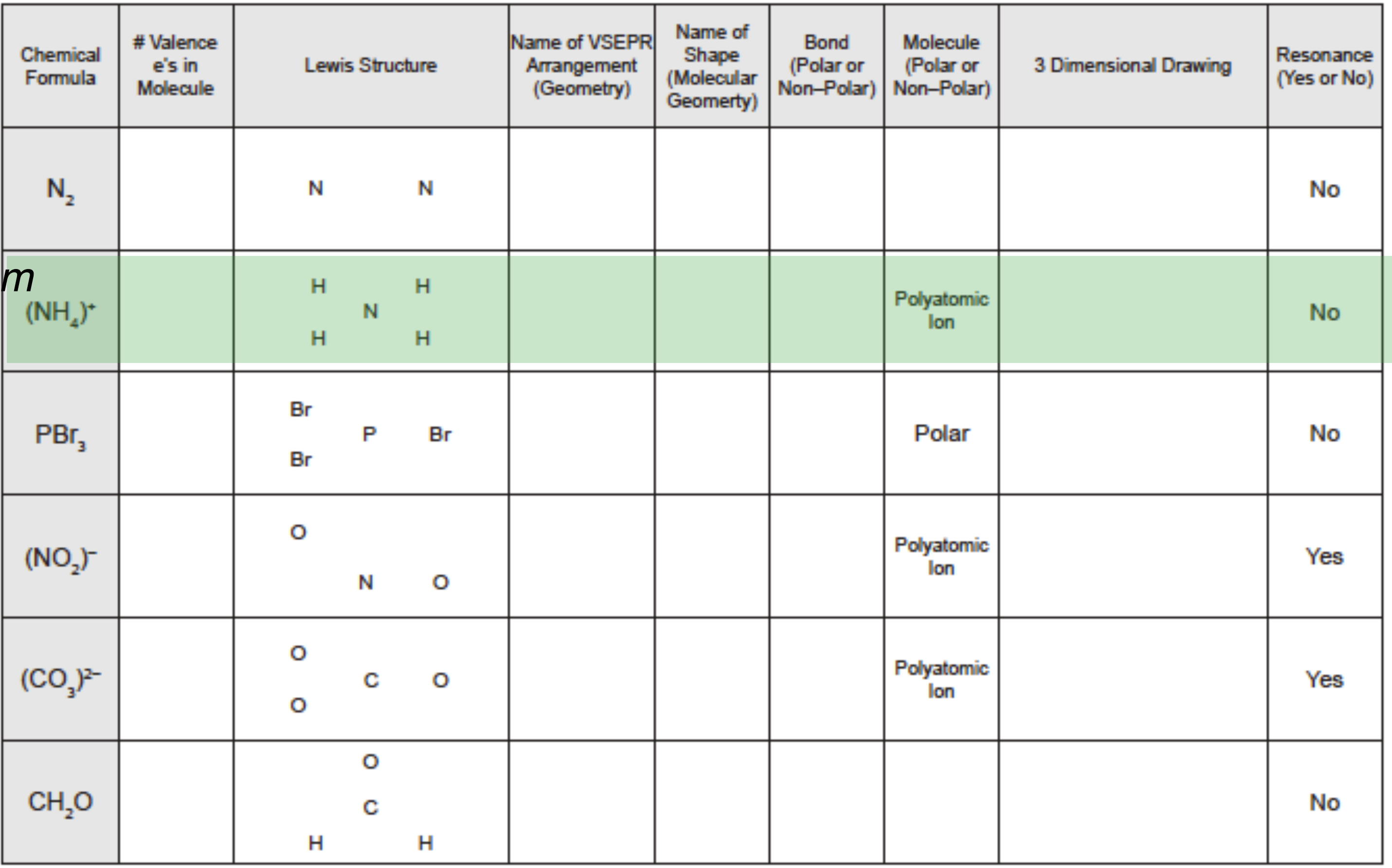


Bonding, Lewis Structures, Molecular Modeling:
Computational Experiments

http://molview.org

Molecular Shapes → Lewis Structures

Ammonium



Chemical Formula	# Valence e's in Molecule	Lewis Structure	Name of VSEPR Arrangement (Geometry)	Name of Shape (Molecular Geomerty)	Bond (Polar or Non–Polar)	Molecule (Polar or Non–Polar)	3 Dimensional Drawing	Resonance (Yes or No)
N_2		N N						No
$(NH_4)^+$		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

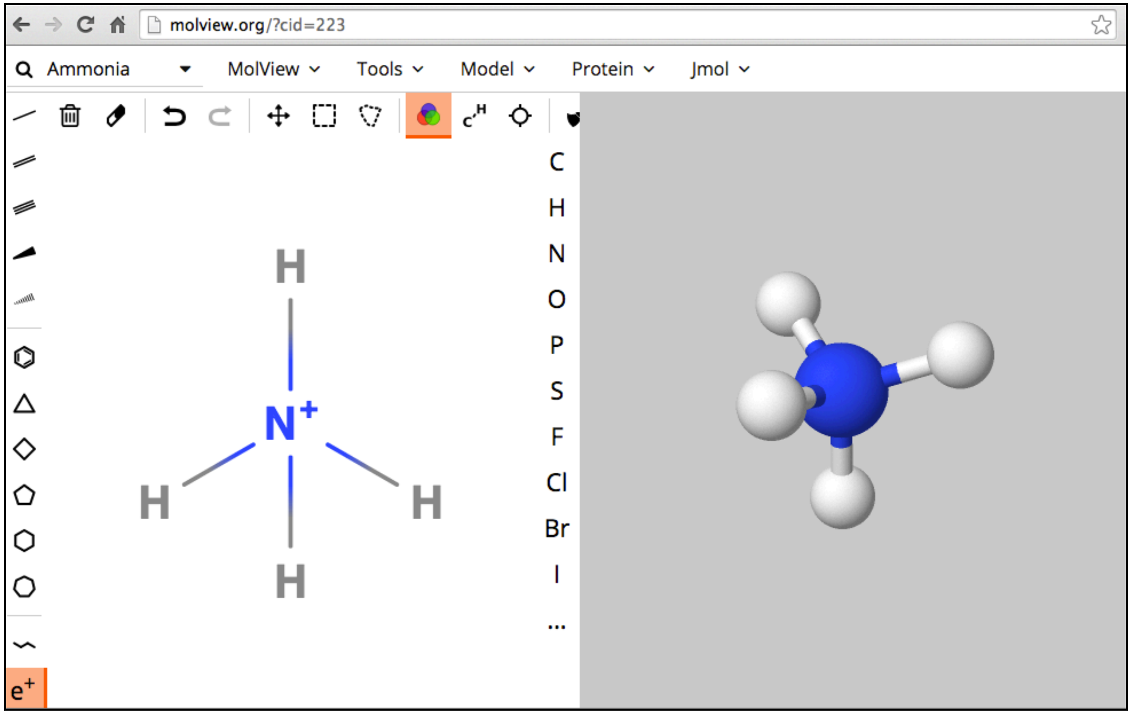
Computational Chemistry: Molecular Modeling Report Form

http://molview.org

Molecular Shapes → Lewis Structures

MolView: Visual On-line Molecular Modeling

build ammonium



Molecular Modeling: Bonding & Lewis Structures

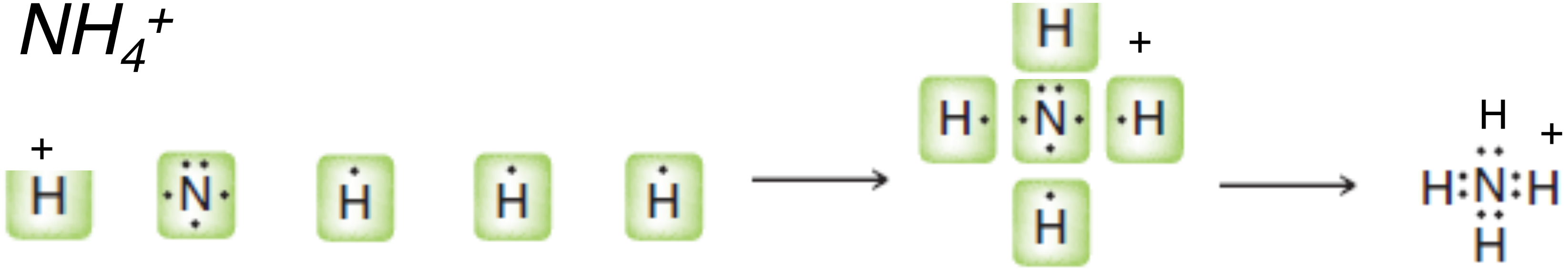
Computational Chemistry: Molecular Modeling Report Form

Lewis Structures → Molecular Shapes

For simple Lewis structures:

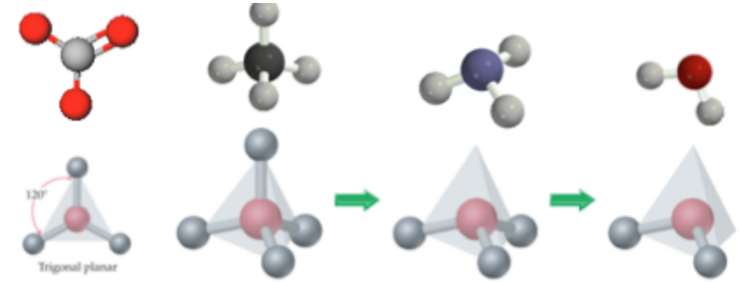
1. *Draw the individual atoms using dots to represent the valence electrons.*
2. *Put the atoms together so they share PAIRS of electrons to make complete octets.*

NH_4^+



Ammonium

Trigonal Planar Tetrahedral Trigonal Pyramidal Bent



Trigonal Planar Tetrahedral Tetrahedral Tetrahedral

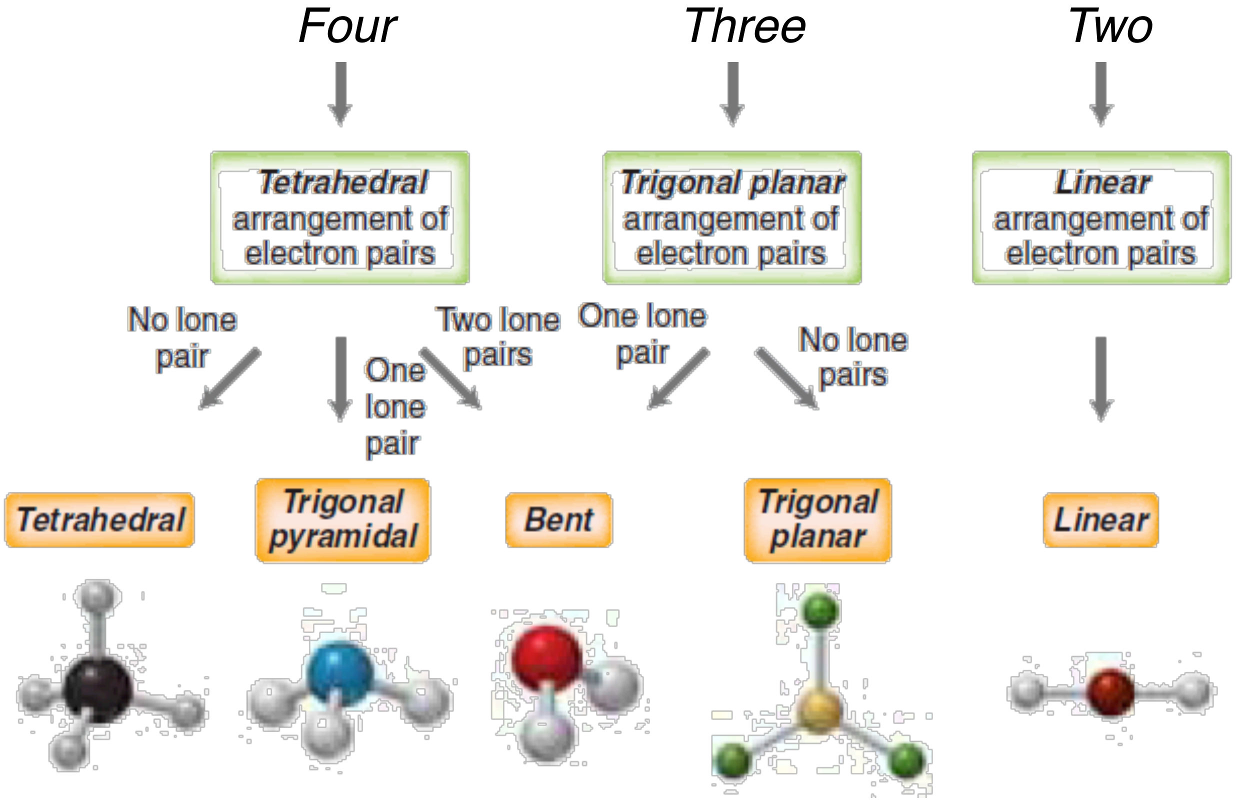
molecular

electronic
(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		

Molecular Geometry – Overview

Numbers of atoms or ("lone" / "free") pairs of electrons about the central atom from Lewis Structure



Four

Three

Two

Tetrahedral arrangement of electron pairs

Trigonal planar arrangement of electron pairs

Linear arrangement of electron pairs

No lone pair

One lone pair

Two lone pairs

One lone pair

No lone pairs

Tetrahedral

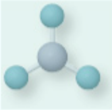
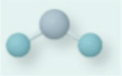
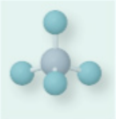
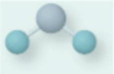
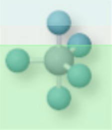
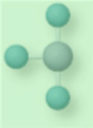
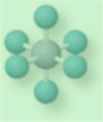
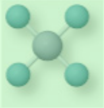
Trigonal pyramidal

Bent

Trigonal planar

Linear

Molecular Geometry Assignment

	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

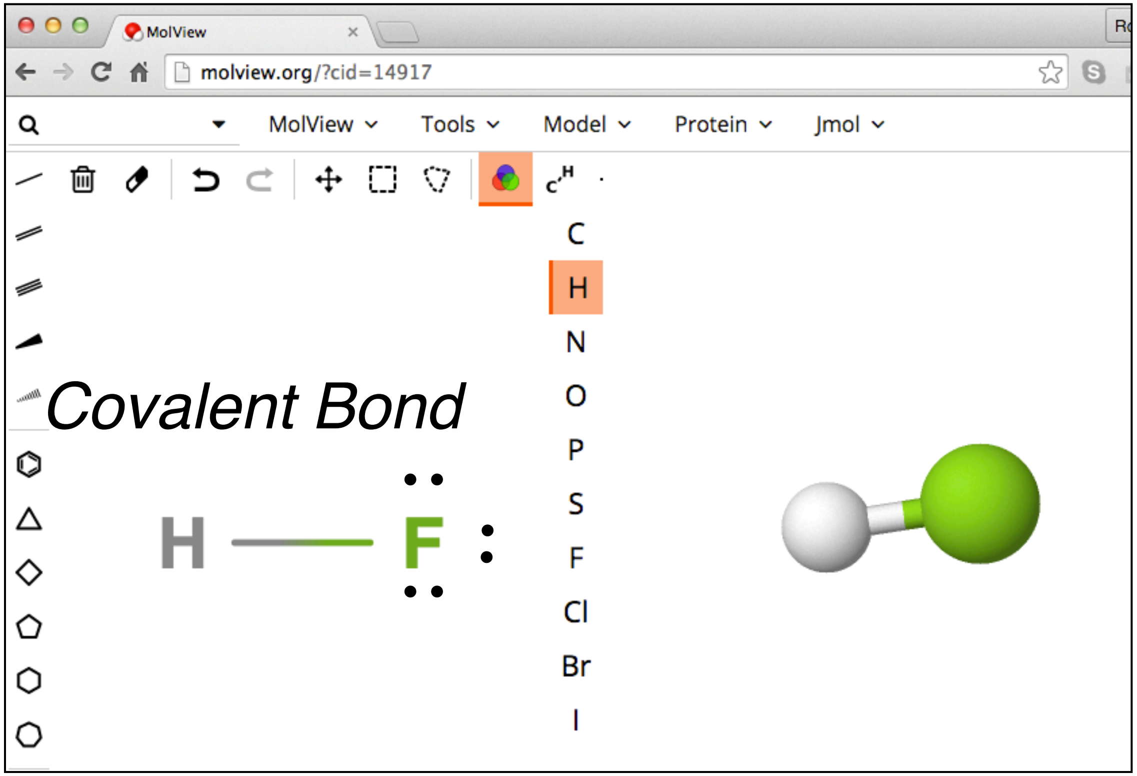
Molecular Modeling
Computational Chemistry

Shapes → Molecular Polarity

Dr. Ron Rusay

Computational Chemistry

Polarity



Covalent Bond

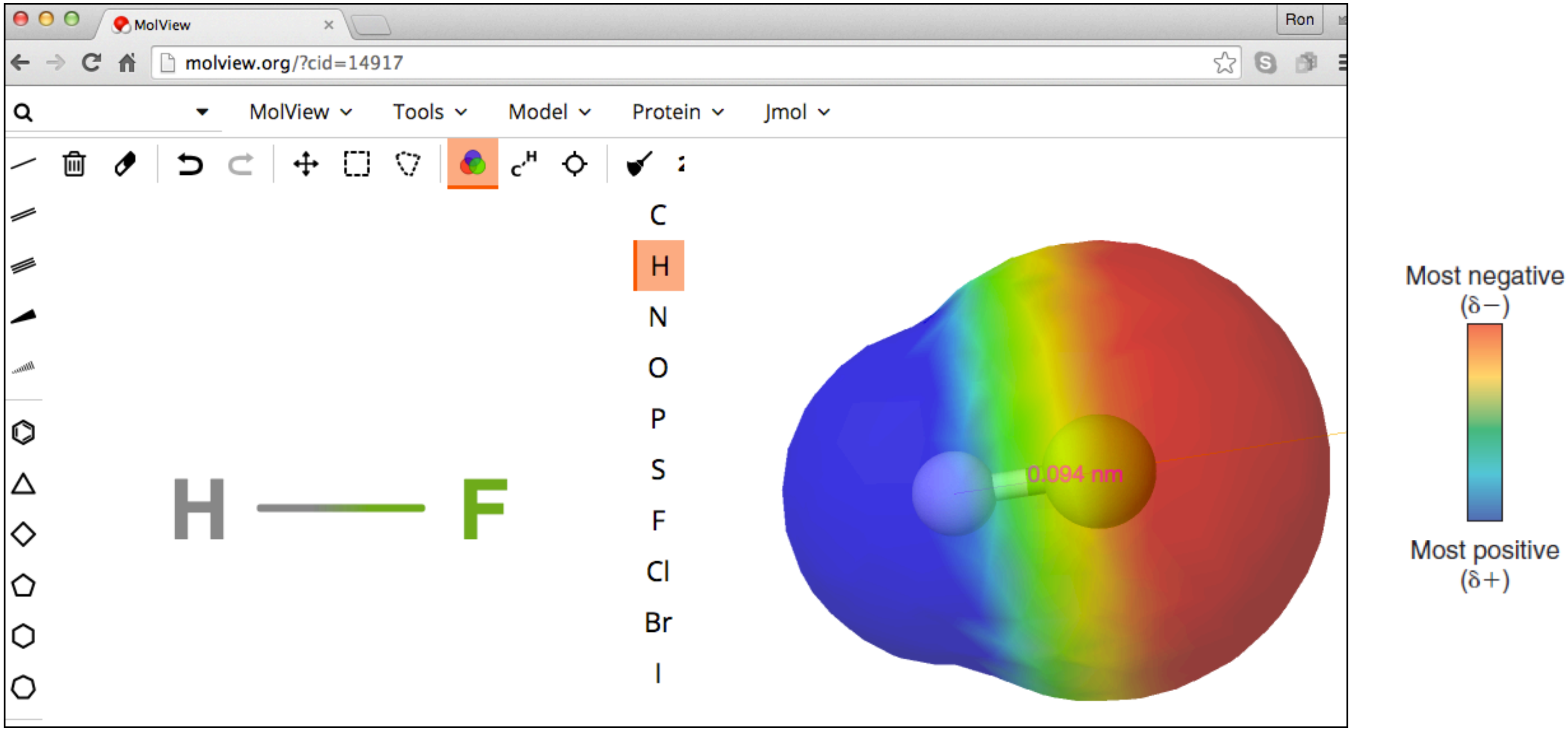
From Jmol dropdown menu click

MEP surface lucent

http://molview.org

Covalent Bonded Compounds

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

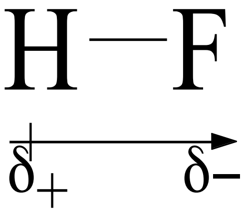


Color coded electron density distribution scale: red-highest δ-, blue highest δ+, green balanced

NOTE: These colors may vary from model to model.

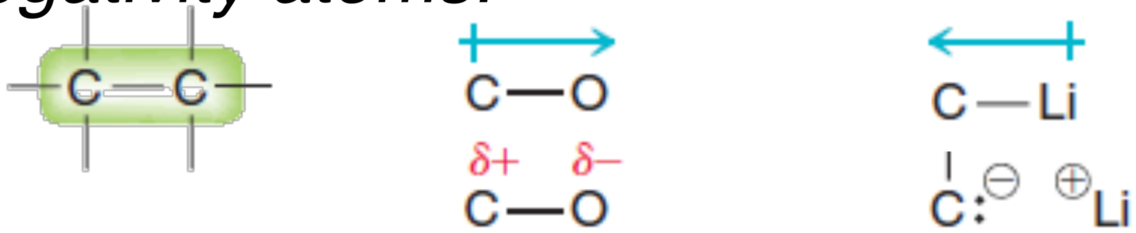
Bond Polarity

A molecule, such as HF, that has a center of positive charge and a center of negative charge is polar; It has a “dipole moment”. The partial charge is represented by δ and the polarity with a vector arrow.

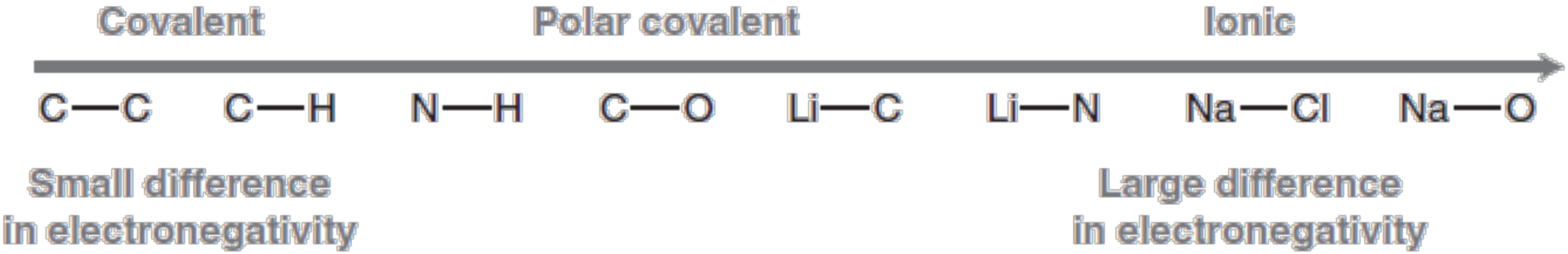


Polar Covalent Bonds

- *Orbital electron density tends to shift away from lower electronegativity atoms to higher electronegativity atoms.*

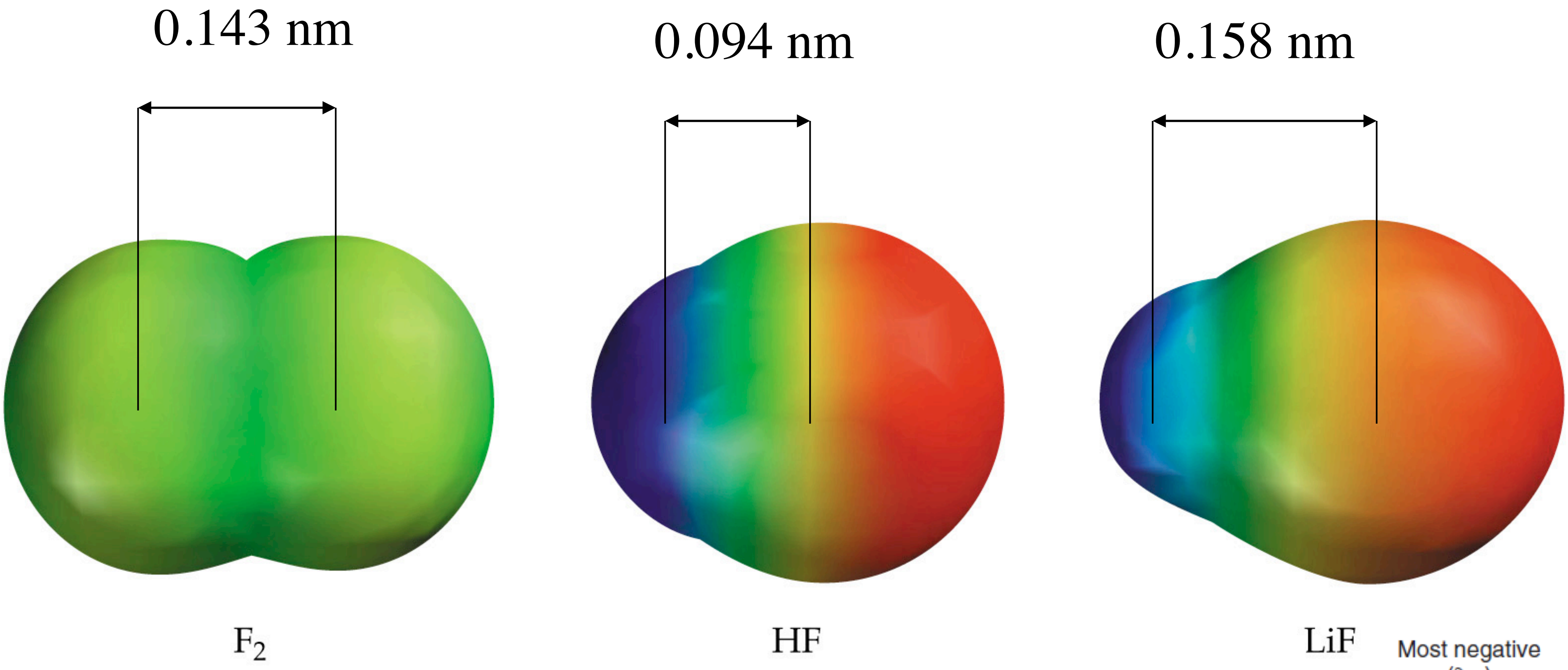


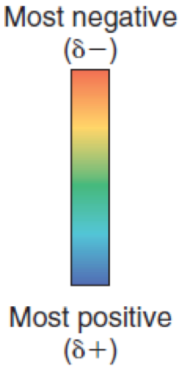
- *The greater the difference in electronegativity, the more polar the bond.*



- *The shorter the bond, the more polar the bond.*

Polarity /Visual Portrayal

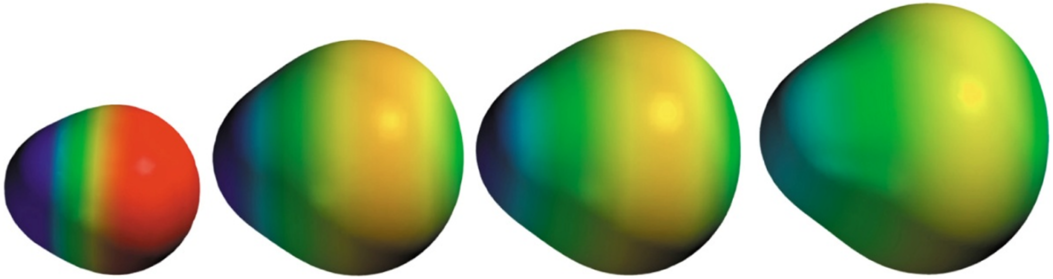




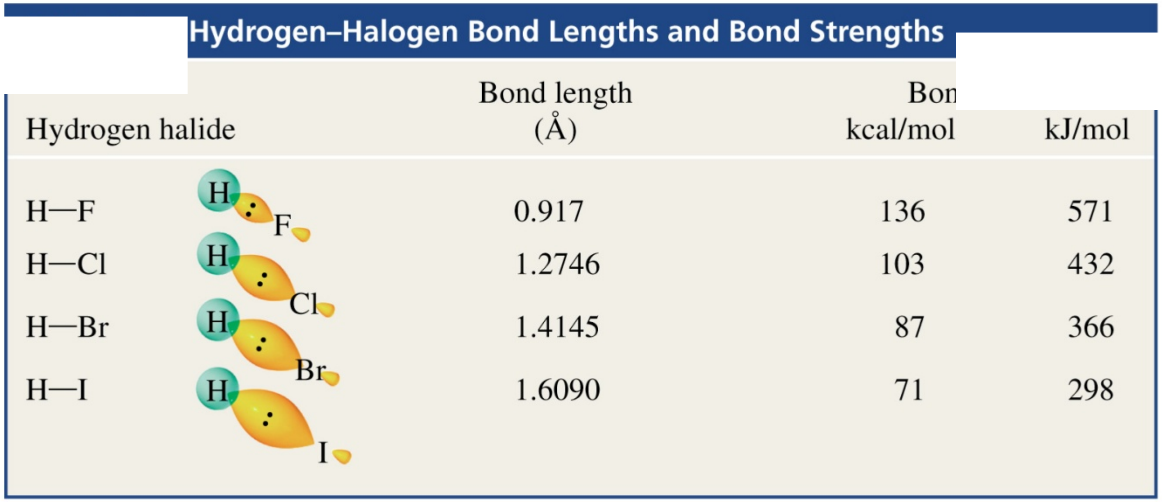
Color coded electron density distribution: blue-lowest, red highest, green balanced

NOTE: These colors do vary.

Hydrogen Halides



What happens to the electronegativities, bond lengths and bond energies going down the column of halogens?



Hydrogen–Halogen Bond Lengths and Bond Strengths

		Bond length (Å)	Bon	
Hydrogen halide			kcal/mol	kJ/mol
H—F		0.917	136	571
H—Cl		1.2746	103	432
H—Br		1.4145	87	366
H—I		1.6090	71	298

Question

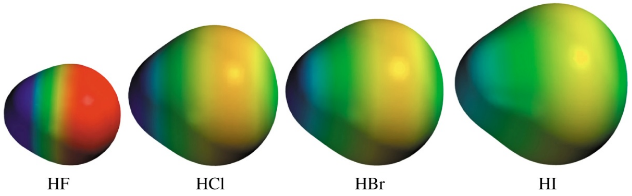
Which of the following bonds is the most polar?

A) H—F

B) H—Cl

C) H—Br

D) H—CH_3



Question

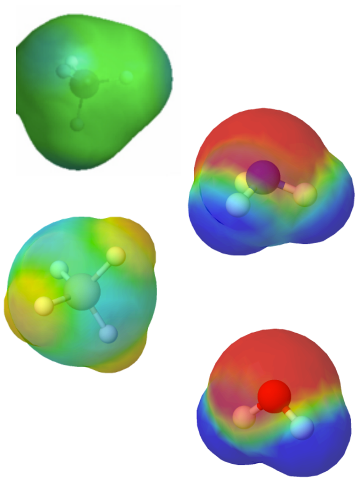
In which of the compounds below is the δ^+ for Hydrogen (H) the greatest?

A) CH_4

B) NH_3

C) SiH_4

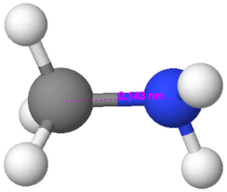
D) H_2O



Question

Which of the following nitrogen bonds is the most polar?

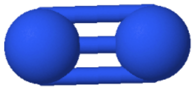
A)



$\mathrm{C-N}$

0.143 nm

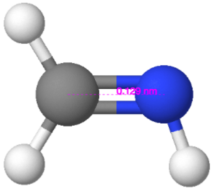
B)



$\mathrm{N\equiv N}$

0.111 nm

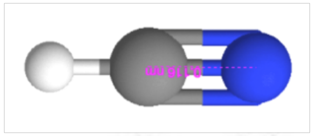
C)



$\mathrm{C=N}$

0.129 nm

D)



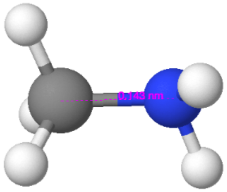
$\mathrm{C\equiv N}$

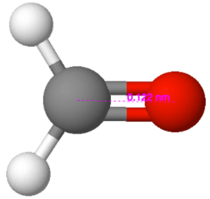
0.116 nm

Bond length: single > double > triple

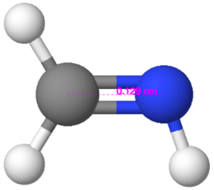
Question

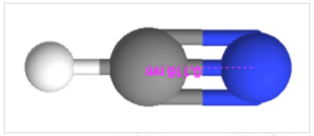
- *Which of the following bonds is the most polar?*





- *A)* $C-N$ *0.143 nm* *B)* $C=O$ *0.122 nm* *2.44D*





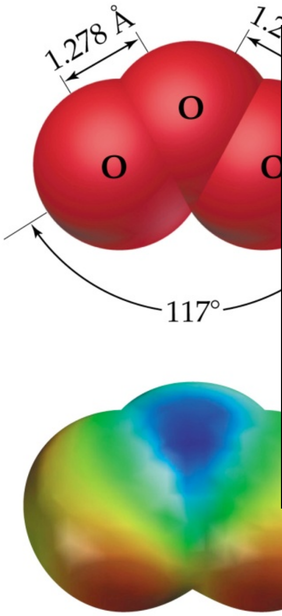
- *C)* $C=N$ *0.129 nm* *D)* $C\equiv N$ *0.116 nm* *3.05D*

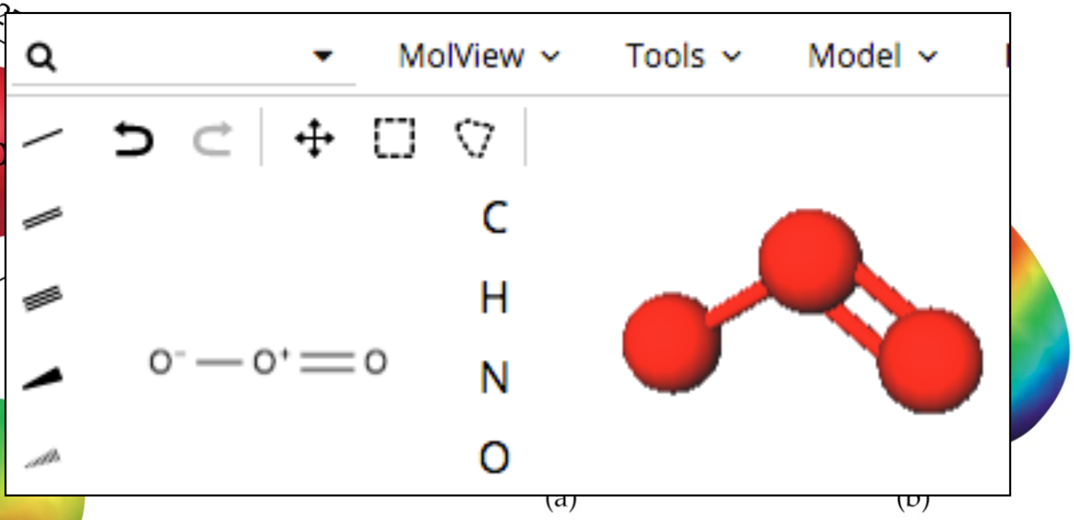
Bond length: single > double > triple

Polarity & Physical Properties

Ozone and Water

0.1278 nm



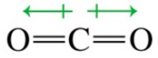


- *Resultant Molecular Dipoles > 0*
- *Solubility: Polar molecules that dissolve or are dissolved in like molecules*

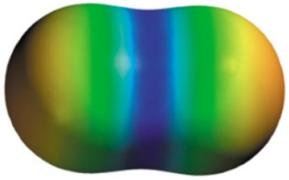
- *The Lotus flower*
- *Water & dirt repellancy: solubility?*

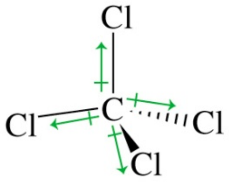
Molecular Polarity

The vector sum of the magnitude and the direction of the individual bond dipoles determine the overall polarity (dipole moment) of a molecule

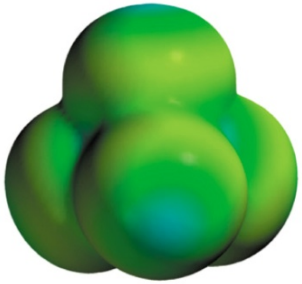


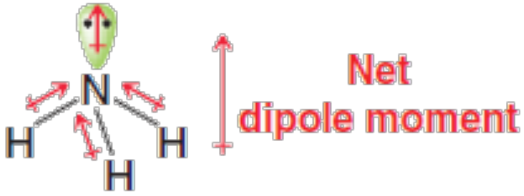
carbon dioxide
$\mu = 0$ D

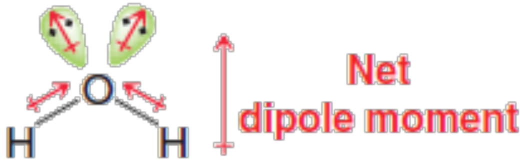


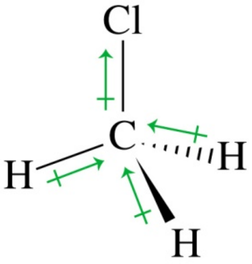


carbon tetrachloride
$\mu = 0$ D

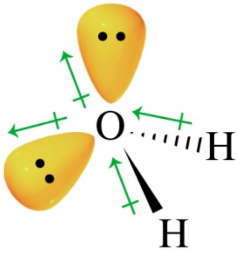




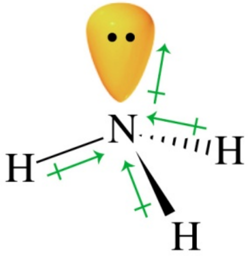




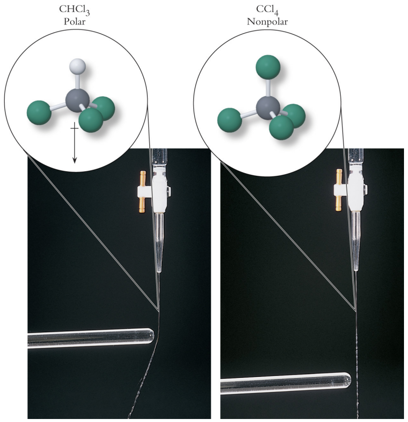
chloromethane
$\mu = 1.87$ D



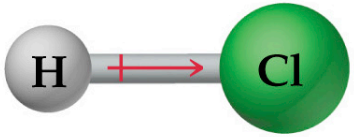
water
$\mu = 1.85$ D



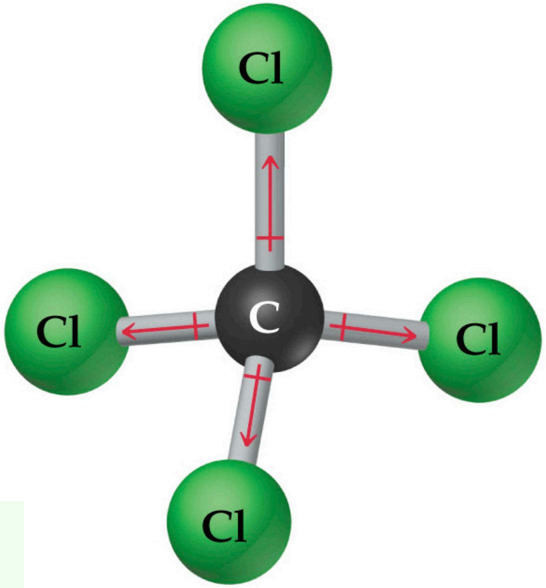
ammonia
$\mu = 1.47$ D



Molecular Polarity

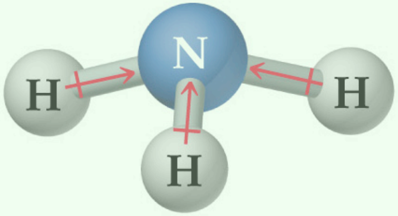


Polar



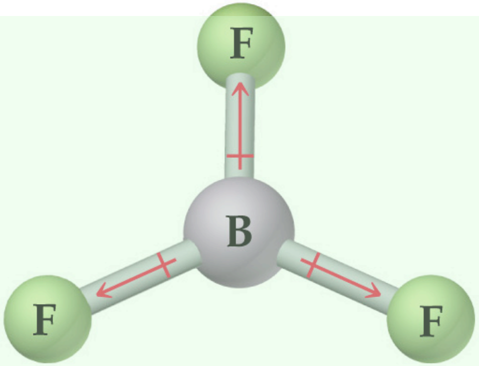
Nonpolar

Tetrahedral



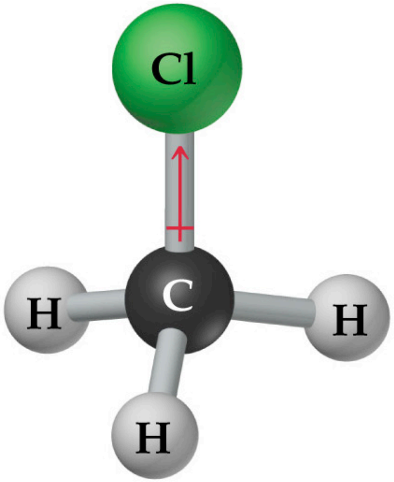
Polar

Trigonal Pyramid



Nonpolar

Trigonal Planar

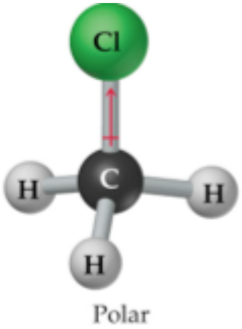


Polar

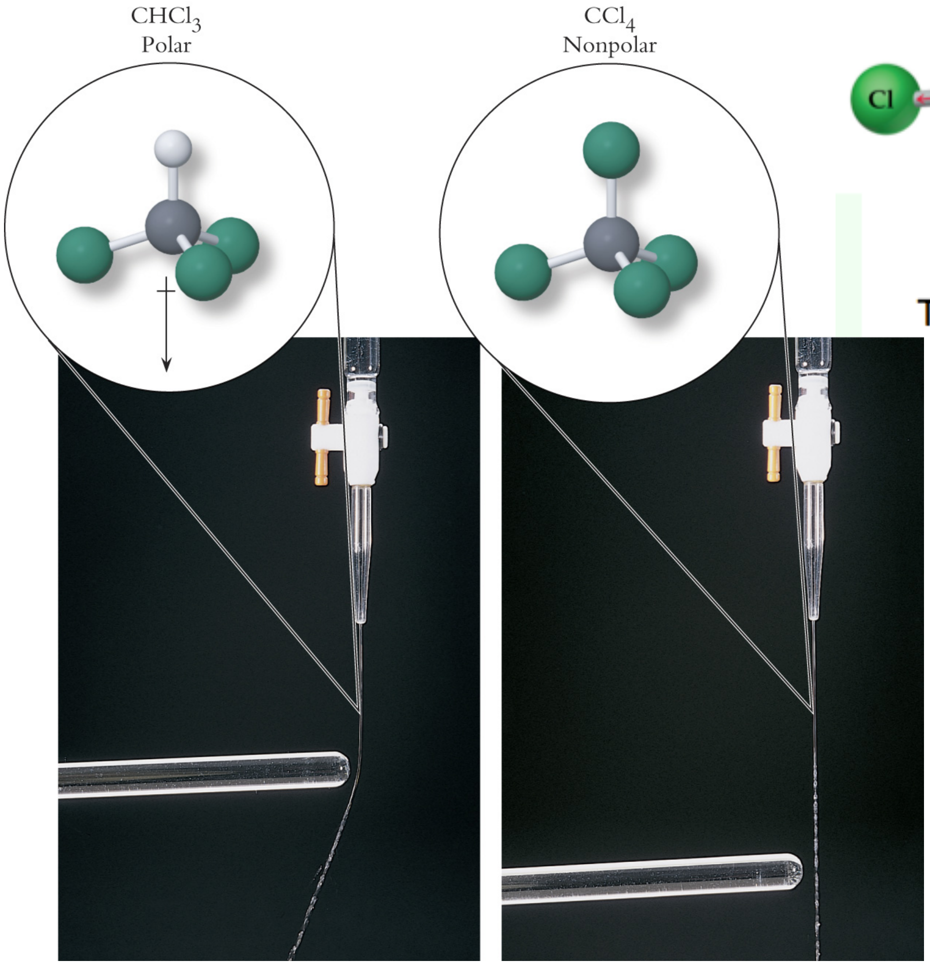
Tetrahedral

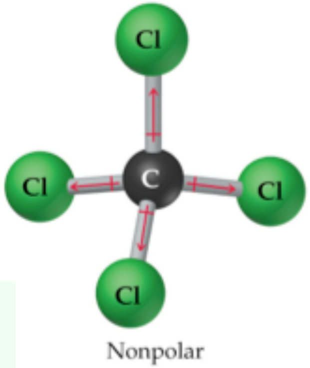
http://chemconnections.org/COT/VSEPR1/

DVC Student Project Group



Tetrahedral





Tetrahedral

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

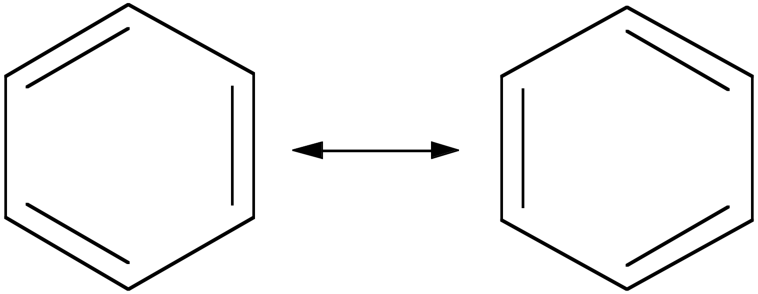
Molecular Modeling
Computational Chemistry

Lewis Structures → Resonance

Dr. Ron Rusay

Resonance

Considered when more than one valid Lewis structure can be written for a molecule without changing the atoms' positions. It is used to explain variations in bond lengths and chemical behavior.

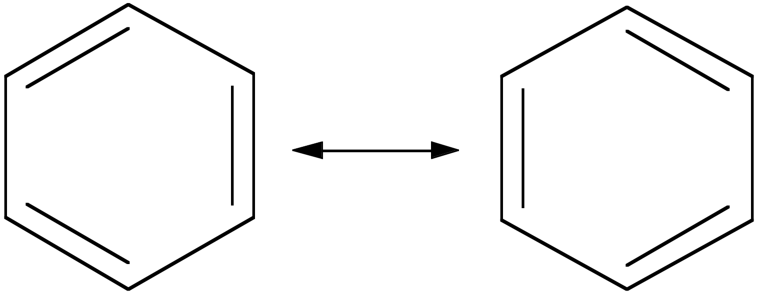


These are shorthand structures.

Each point of an angle in the hexagon equals a carbon atom, the hydrogen atoms are not shown & must be deduced from the fact that carbon forms 4 bonds.

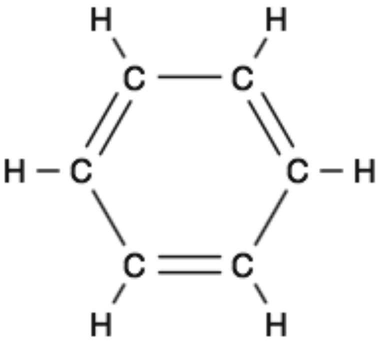
Shorthand

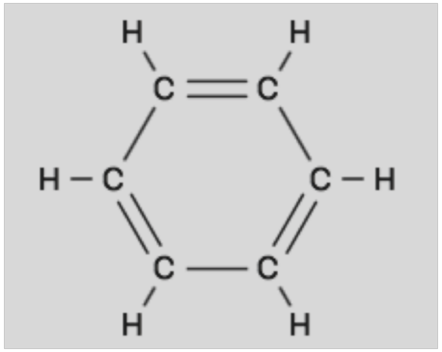
“Bond Line”Structures



Each point of an angle in the hexagon equals a carbon atom, the hydrogen atoms are not shown & must be deduced from the fact that carbon forms 4 bonds.

C_6H_6

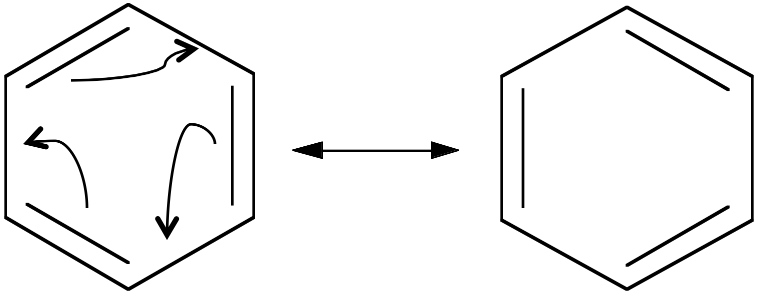




C_6H_6

Resonance

Moving electrons:



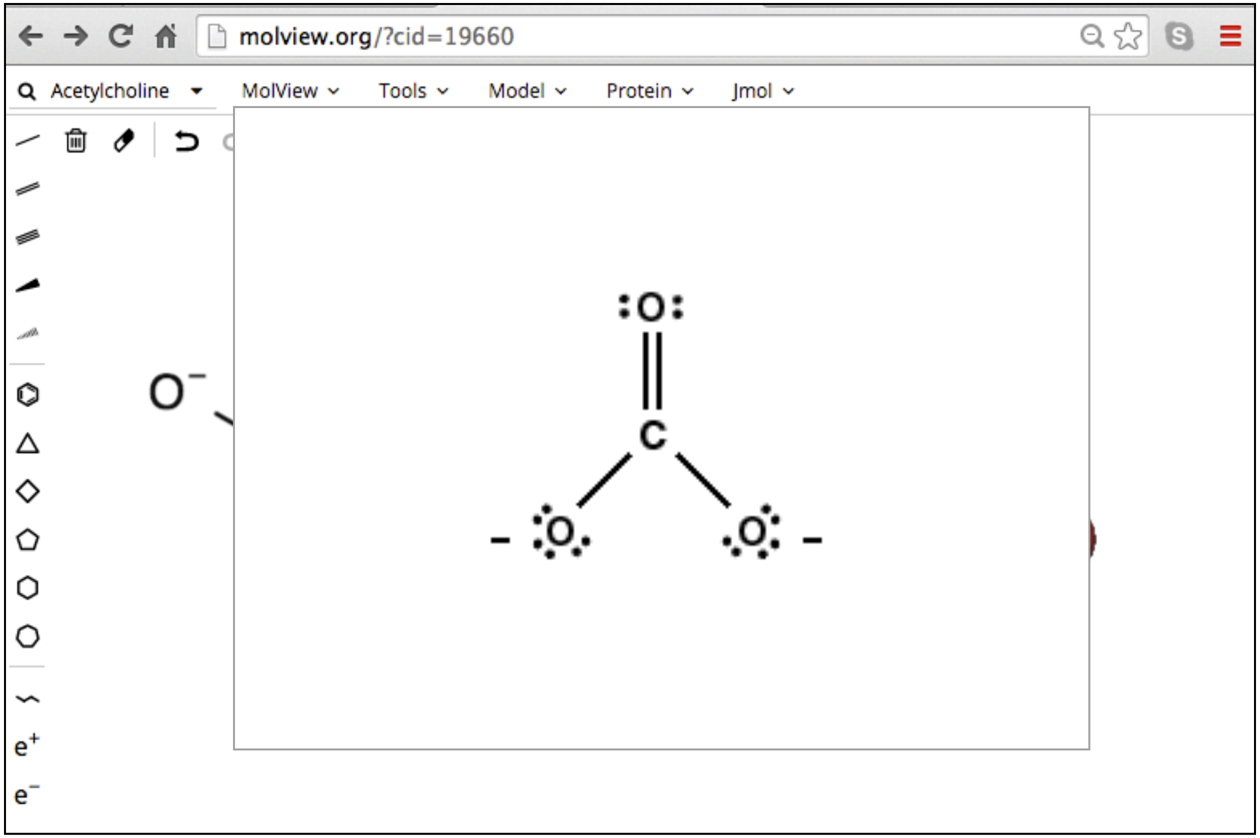
The overall structure is considered to be a weighted average of all of the possible valid Lewis structures where some are more favored than others.

Resonance structures are mental images used to explain the observed arrangement of the atoms and their bond lengths and bond angles.

http://molview.org

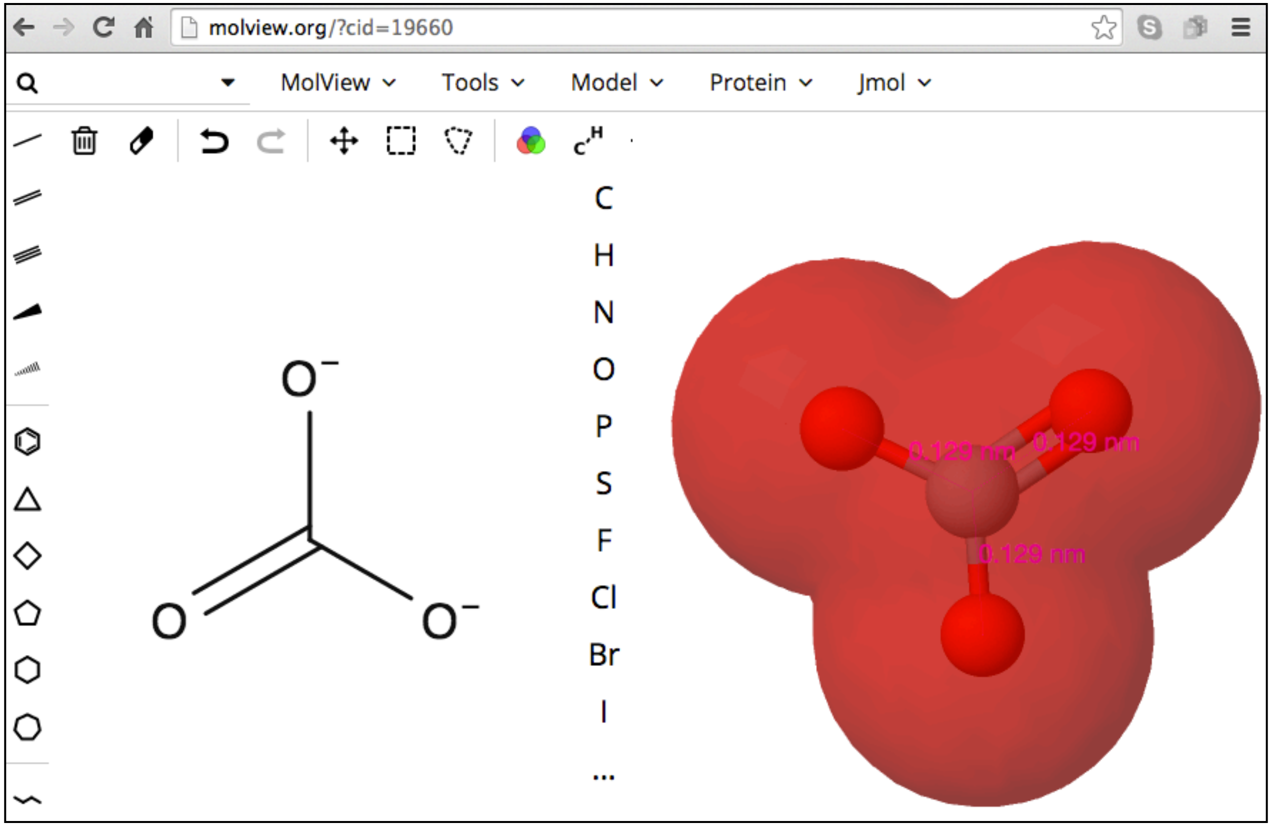
Molecular Shapes ⟷ Lewis Structures

MolView: Polyatomic Ions



Bonding, Lewis Structures, Molecular Modeling:

Carbonate Ion Resonance



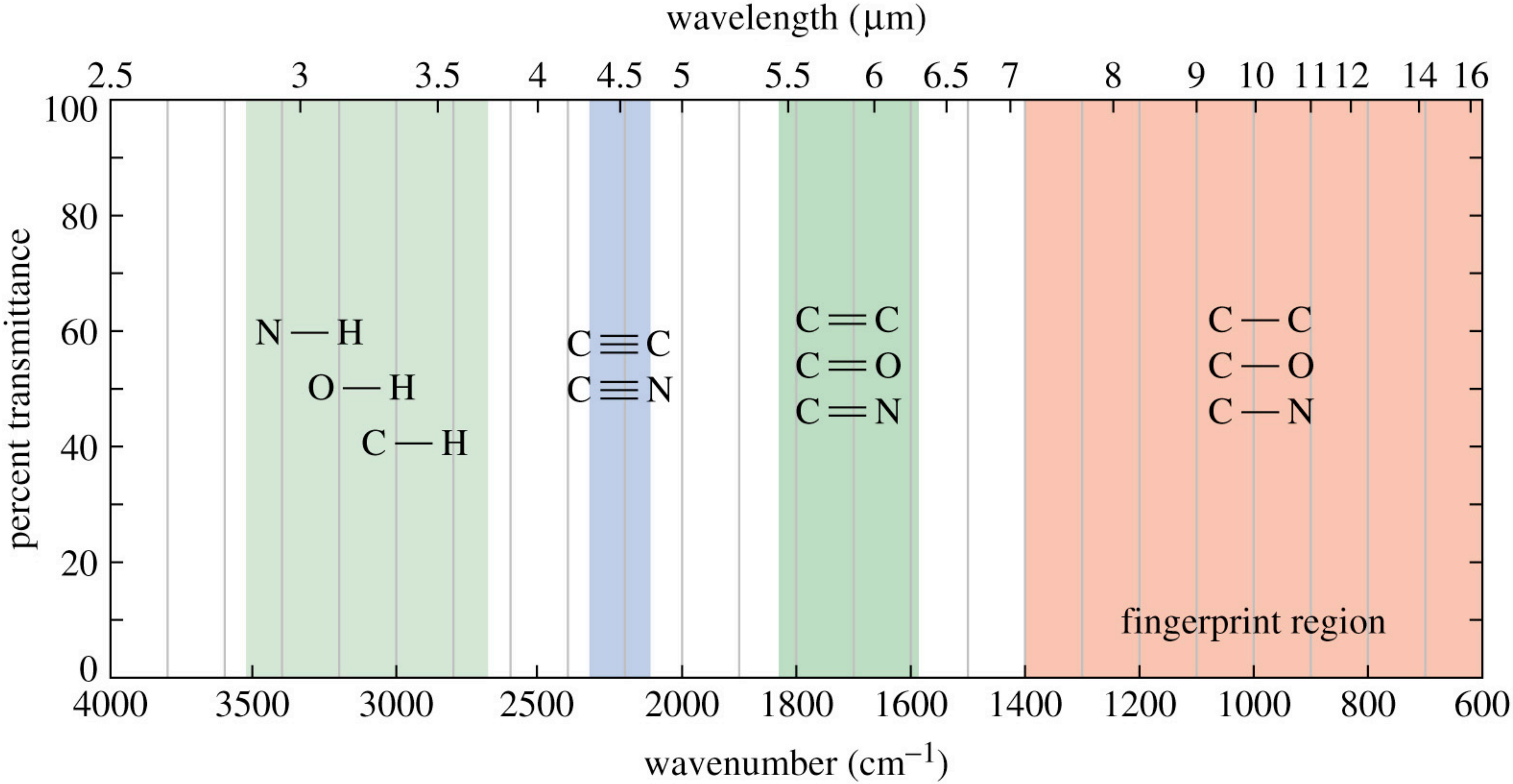
The 3-d structure is an average of the resonance structures. The normal bond length of a C=O bond is ~0.120 nm and C-O is ~0.142 nm.

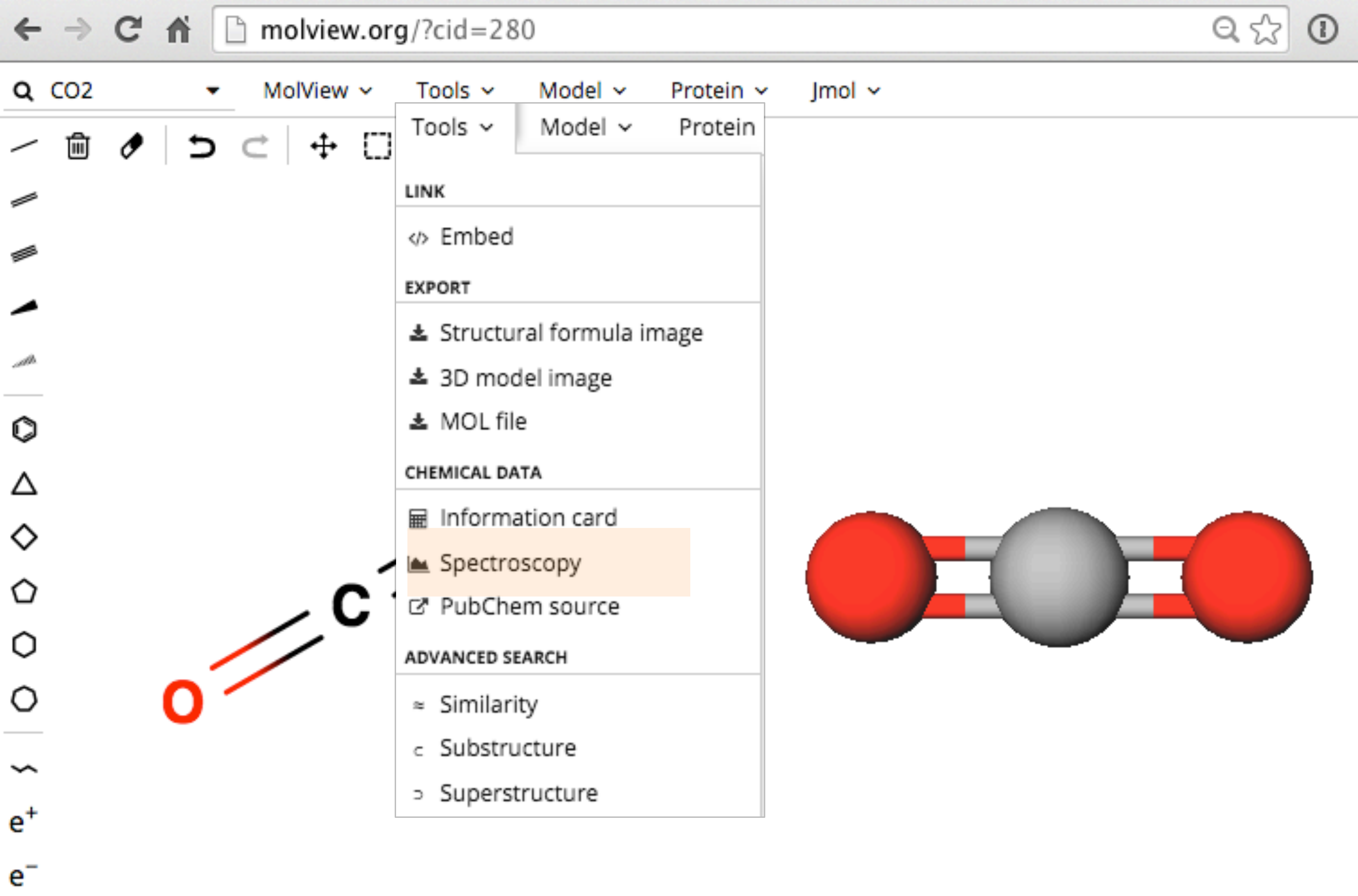
Molecular Modeling
Computational Chemistry

Molecular Energy Absorbance

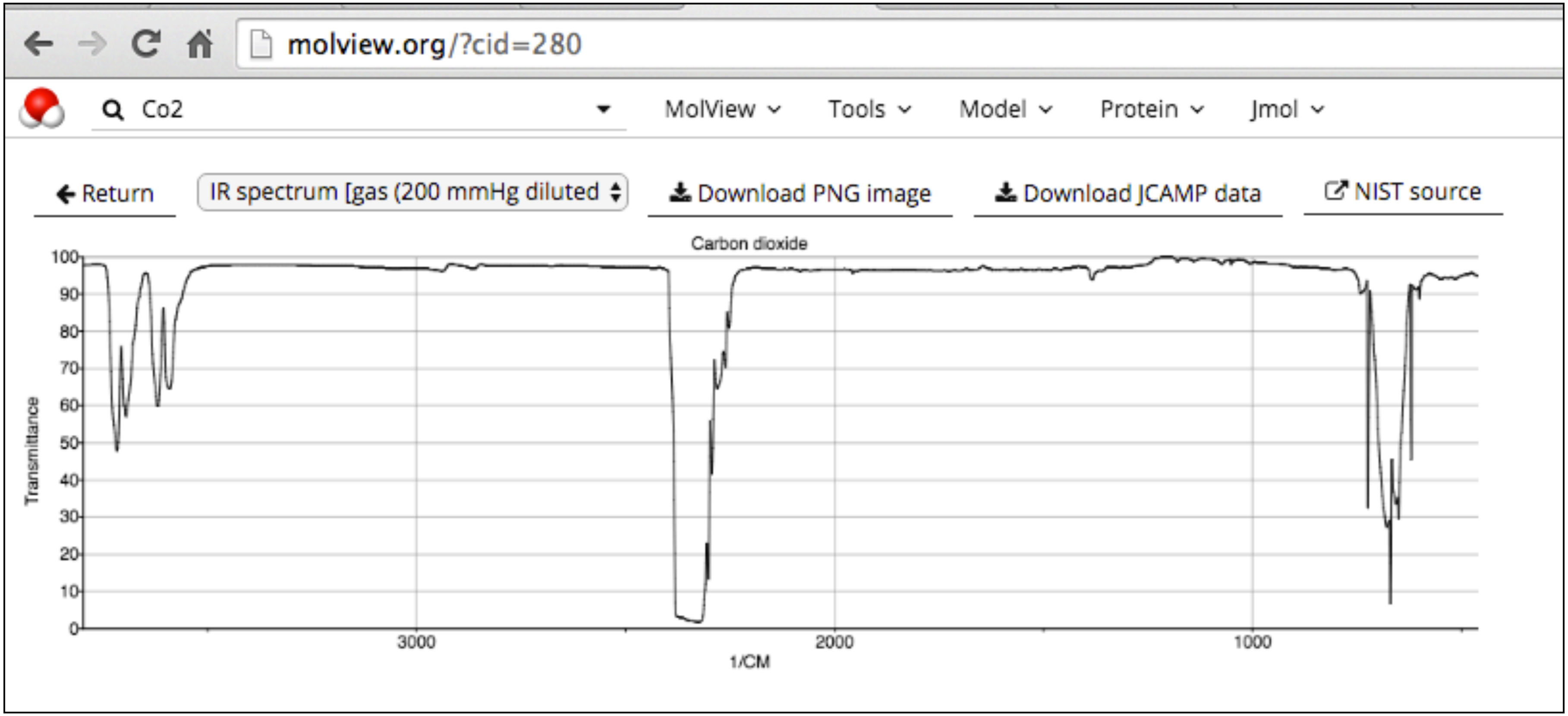
Dr. Ron Rusay

Infrared Energy - Bond Absorbances




molview.org/?cid=280
CO2
MolView
Tools
Model
Protein
Jmol
Tools
Model
Protein
LINK
Embed
EXPORT
Structural formula image
3D model image
MOL file
CHEMICAL DATA
Information card
Spectroscopy
PubChem source
ADVANCED SEARCH
Similarity
Substructure
Superstructure
C
O
e+
e−

Infrared- Bond Absorbances



molview.org/?cid=280

Co2

IR spectrum [gas (200 mmHg diluted

[*http://molview.org*](http://molview.org)

Infrared- Bond Absorbances

Atmospheric CO_2

September 2018

405.51

parts per million (ppm)

Mauna Loa Observatory, Hawaii (NOAA-ESRL)

Preliminary data released **October 5, 2018**

https://www.co2.earth/