

Molecular Modeling Computational Chemistry

Lewis Structures, Bonds, Shapes,
Polarity, Stereochemistry

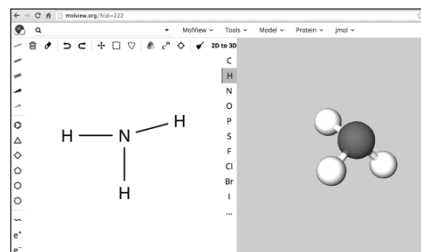
Molview: Ancillary Materials & Questions



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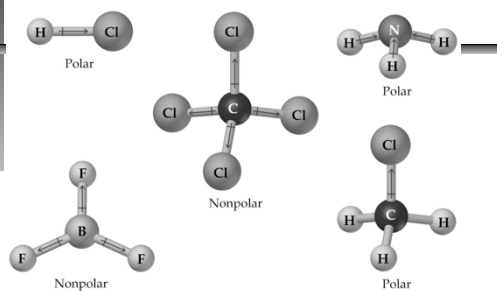
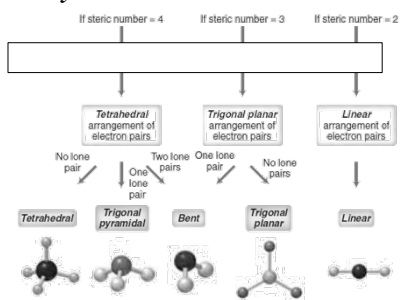
<http://molview.org>

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



Bonding, Lewis Structures, Molecular Modeling:
Computational Experiments, Instructions, & Manual pp. 53-58

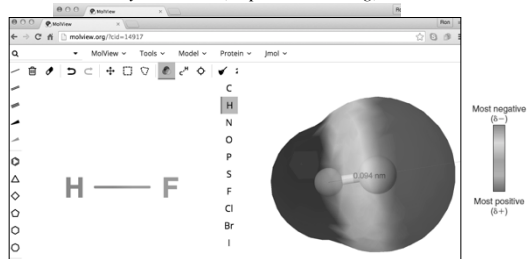
Molecular Geometry – Summary



<http://chemconnections.org/COT/VSEPR1/>
DVC Student Project Group

Computational Chemistry

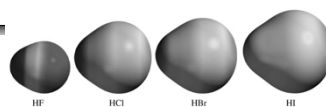
Polarity: Molview (<http://molview.org>)



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

NOTE: These colors may vary from model to model.

Hydrogen Halides



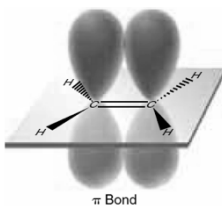
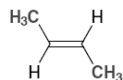
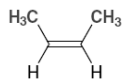
Hydrogen-Halogen Bond Lengths and Bond Strengths				
Hydrogen halide	Bond length (Å)	Bond strength		
		kcal/mol		kJ/mol
H-F	0.917	136		571
H-Cl	1.2746	103		432
H-Br	1.4145	87		366
H-I	1.6090	71		298

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

Stereochemical cis-trans Isomers

- To maintain orbital overlap in the π bond, $C=C$ double bonds cannot freely rotate.

- Although the two molecules below have the same connectivity, they are NOT identical.



Chemical Communication



<http://chemconnections.org/organic/chem226/Labs/Smell/ChemComm.html>

Pheromone Synthesis
[20:40-23:51]

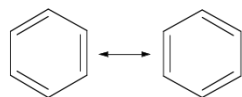


<http://www.learner.org/resources/series61.html>

<http://chemconnections.org/general/movies/pheromones-IR.mov>

Resonance

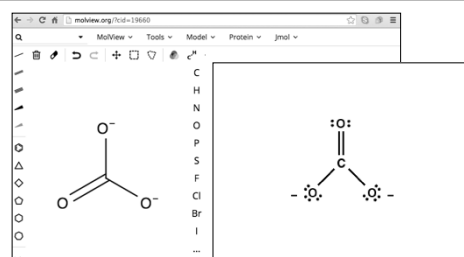
Considered when more than one valid Lewis structure can be written for a molecule without changing the atoms' positions. Used to explain variations in bond lengths and chemical behavior.



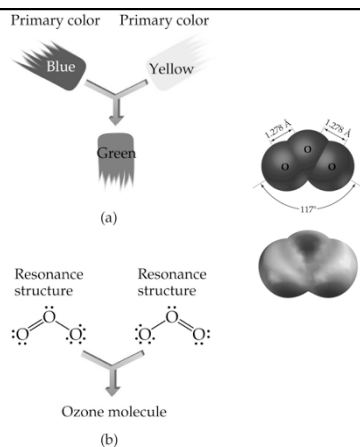
These are resonance structures. The actual structure is considered to be an average of the resonance structures.

<http://chemconnections.org/general/movies/resonance.mov>

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.



Question

Which of the following bonds is the most polar?

- | | |
|-------------------------|---------------------------|
| A) $\text{H}-\text{F}$ | B) $\text{H}-\text{Cl}$ |
| C) $\text{H}-\text{Br}$ | D) $\text{H}-\text{CH}_3$ |

Answer

Which of the following bonds is the most polar?

- A) H—F B) H—Cl
C) H—Br D) H—CH₃

Question

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

- A) CH₄
B) NH₃
C) SiH₄
D) H₂O

Answer

► In which of the compounds below is the δ^+ for H the greatest?

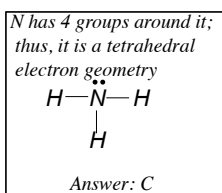
- A) CH₄
► B) NH₃
► C) SiH₄
► D) H₂O

What shape is water?

- a. Tetrahedral
b. **Bent**
c. Trigonal planar
d. Linear

What is the electronic geometry of NH_3 ?

- a. Linear
- b. Trigonal Planar
- c. Tetrahedral
- d. Trigonal Pyramidal

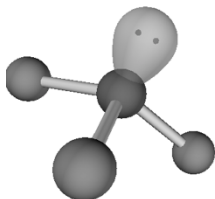


Which of these molecules has a linear molecule geometry?

- a. CO_2
- b. O_3
- c. Both
- d. Neither

Which molecule could be represented with this diagram?

- a. BH_3
- b. CH_4
- c. NH_3



What is the molecular geometry of H_2S ?

- a. Linear
- b. Tetrahedral
- c. Trigonal pyramidal
- d. Bent

