Slide 1

Molecular Modeling
Computational Chemistry

Molecular Shapes, Polarity

Dr. Ron Rusay

Slide 2

Shapes of Molecules

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

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

Slide 3

Shapes of Molecules

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

Slide 4

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

❥ Fundamental repeating shapes found in every biological molecule
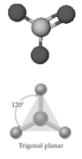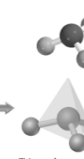
C = black
H = gray
N = blue
O = red

pink = generic atom

Slide 5

http://molview.org
Molecular Shapes → Lewis Structures

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)
H₂O		O H H				Polar		No
NH₃		H N H H				Polar		No
CH₄		H H H C H H						No
C₂H₄		H C C H 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
C₂H₂		H C C H	Around each C	Around each C	C–H C–C			No
SO₃		O S O O				Non-Polar		Yes

Molecular Modeling: Bonding & Lewis Structures
Computational Chemistry: Molecular Modeling Report Form
Replaces Lab Manual pp. 53-58

Slide 6

http://molview.org
Molecular Shapes → Lewis Structures
MolView: Visual On-line Molecular Modeling

Ammonia

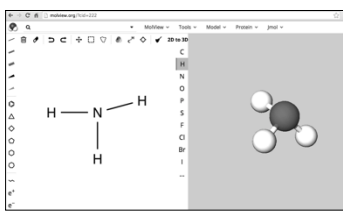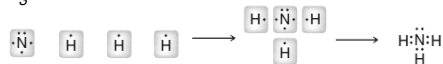*Molecular Modeling: Bonding & Lewis Structures*
Computational Chemistry: Molecular Modeling Report Form
Replaces Lab Manual pp. 53-58
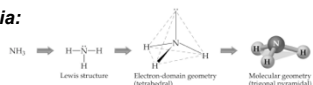
Lewis Structures → Molecular Shapes

- *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

Ammonia:

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
$(NH_4)^+$		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

Ammonium

Molecular Modeling: Bonding & Lewis Structures
Computational Chemistry: Molecular Modeling Report Form
Replaces Lab Manual pp. 53-58

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

Ammonium

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Lewis Structures → Molecular Shapes

- *For simple Lewis structures:*
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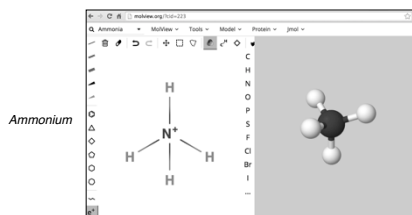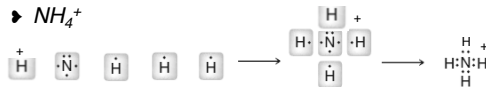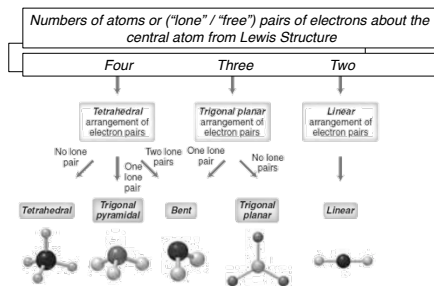 2. Put the atoms together so they share PAIRS of electrons to make complete octets.
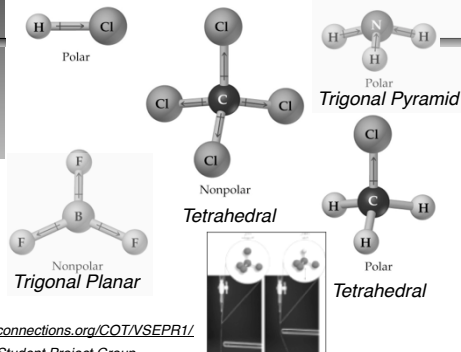- NH_4^+

Ammonium

Molecular Geometry – Overview

Molecular Geometry Assignment

Molecular Polarity

DVC Student Project Group

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

O=C=O
carbon dioxide
$\mu = 0$ D

Cl
Cl—C—Cl
carbon tetrachloride
$\mu = 0$ D

N
H H H
Net dipole moment

O
H H
Net dipole moment

Cl
H—C—H
H
chloromethane
$\mu = 1.87$ D

O
H H
water
$\mu = 1.85$ D

N
H H H
ammonia
$\mu = 1.47$ D