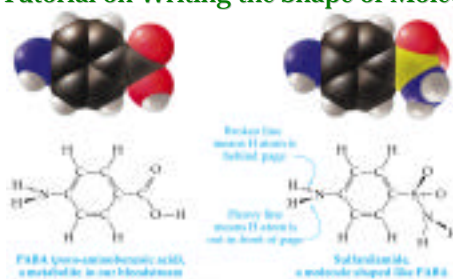


Constructing Molecular Shapes

A Tutorial on Writing the Shape of Molecules



Dr. Fred Omega Garces
Chemistry 100
Miramar College



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Determining Molecular Shape

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VSEPR- Valence Shell Electron-Pair Repulsion Theory

Main premise of model-

Valence electron pair repel each other in molecule with shapes the molecule

Molecule assumes Geometry that minimizes electrostatic repulsion:

Occurs when electron pair are far apart as possible.

Driving force is the Pauli exclusion principle :

2 electrons with same spin can't occupy the same space.

Electronic Geometry is the geometry around the central atom in which electron-electron repulsion is minimize.

AE_n (system)

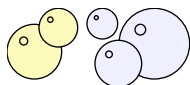
Molecular Geometry is geometry around central atom when electron pairs are replace by bonding atoms and the nonbonding electrons are ignored.

AB_mE_n (system)

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VSEPR- Procedural Steps



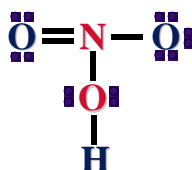
1) Determine the **Lewis Structure**.



- Valence electrons for each atom in the structure.
- Determine the atomic sequence, the number of bonds, remaining electrons
- Write Lewis structure with each atom obeying the octet rule



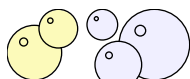
Example: HNO_3 (See [Lewis Structure Tutorial](#))



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VSEPR- Procedural Steps



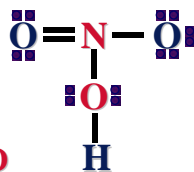
2) Determine **electronic geometry** (AE_n system) from Lewis structure.



- Count the electron domain (region) around the central atom.
- Arrange electron domain to minimize electron-electron repulsion.
Occurs when electron pair are far apart as possible.
- 2-domain \rightarrow linear, 3-domain \rightarrow trigonal, 4-domain \rightarrow tetrahedral



Example: HNO_3



Central Atoms, **N** and **O**

N: Three electron domain

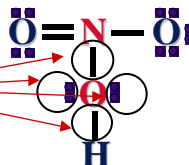
$\text{AE}_3 \rightarrow$ Trigonal

O: Four electron domain

$\text{AE}_4 \rightarrow$ Tetrahedral

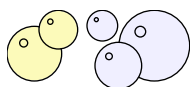


General all electron pairs in Lewis structures are shown as pairs of dots.



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VSEPR- Procedural Steps



3) Determine **molecule geometry** (AB_mE_n) from electronic geometry.

a) The geometry is based on the position of the atoms.

b) The lone pair electrons are ignored for the molecular geometry.

i) Elec Geometry - Linear AE_2 . Molc Geometry-Linear AB_2

ii) Elec Geometry - Trigonal AE_3 . MolcGeo- Trig AB_3 or Bent AB_2E

ii) Elec Geometry - Tetrahedral AE_4 . Molc Geo -tetr AB_4 , pyramid AB_3E or Bent AB_2E_2

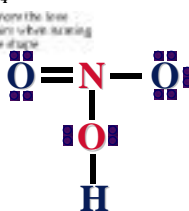


Example: HNO_3

Central atom: **Nitrogen**

Elec Geometry - AE_3 Trigonal.

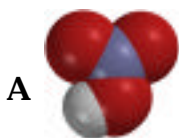
Molc Geometry - AB_3 Trigonal.



Central atom: **Oxygen**

Elec Geometry - AE_4 Tetrahedral

Molc Geometry - AE_2B_2 Bent ("V")

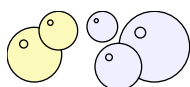


Space Filling Model (A) and Ball and Stick Model (B). The shape around the Nitrogen has a trigonal geometry and the shape around the oxygen is a bent (or "V") shape.

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Determining Molecular Shape

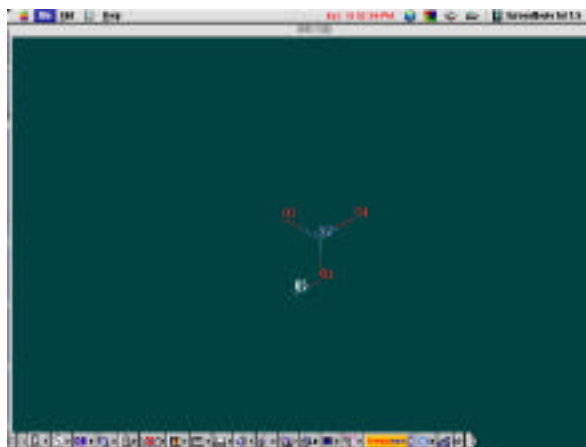
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HNO_3 Quick Time Movie



Click on the movie to start the QuickTime Movie on the perspective of the Nitric acid (HNO_3) molecule.



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Determining Molecular Shape

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VSEPR Table

Electron Groups			Arrangement of Groups	Molecular Shape	Example
Total	Bonding	Lone			
2	2	0	Linear	Linear	CO_2
3	3	0	Trigonal planar	Trigonal planar	NO_3^-
	2	1		Bent (or angular)	O_3
4	4	0	Tetrahedral	Tetrahedral	CH_4
	3	1		Trigonal pyramidal	PF_3
	2	2		Bent (or angular)	H_2O

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Determining Molecular Shape

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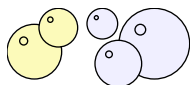
VSEPR Table: QuickTime Movie

Electron Groups			Arrangement of Groups	Molecular Shape	Example
Total	Bonding	Lone			
2	2	0	Linear	Linear	CO_2
3	3	0	Trigonal planar	Trigonal planar	NO_3^-
	2	1		Bent (or angular)	O_3
4	4	0	Tetrahedral	Tetrahedral	CH_4
	3	1		Trigonal pyramidal	PF_3
	2	2		Bent (or angular)	H_2O

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Determining Molecular Shape

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Summary



Key to determine molecular Geometry

- **Lewis Structure**
Determine electron domain in structure.
- **Electronic Geometry**
Establish the AE_n system.
- **Molecular Geometry**
Establish the AB_mE_n system.
Don't count lone pairs in the molecular.

