

SHAPES OF MOLECULES

This handout will help you with understanding the shapes of molecules based on their Lewis structure. The shape of a molecule is determined by minimization of the electron clouds that surround a central atom. The atomic orbitals of the central atom have hybridized, with the hybrid orbitals arranging themselves in the shape that minimizes the repulsions of electrons occupying these hybrid orbitals. If you have trouble drawing Lewis structures, please refer to the handout addressing drawing Lewis structures. We will use the following key to describe the shapes of molecules.

Structure type: A = central atom
X = bonded group (regardless of bond order)
E = electron pair on the central atom

Groups: sum of X and E (number bonded groups and electron pairs)

Hybridization: which atomic orbitals were mixed

Electronic geometry: shape based on regions of electron density

Molecular geometry: shape based on location of nuclei

Bond angle: angle between X-A-X (central atom and two bonded groups)

We will look at each structure type in turn. An example of each will be given.

Compound: CO₂

Structure Type: AX₂

2 groups

2 hybrid orbitals have formed

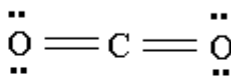
2 atomic orbitals were mixed

Hybridization: sp

Electronic geometry: linear

Molecular geometry: linear

Bond angle: 180°



Compound: H₂CO

Structure Type: AX₃

3 groups

3 hybrid orbitals have formed

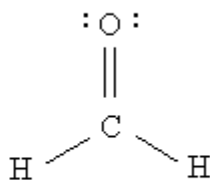
3 atomic orbitals were mixed

Hybridization: sp²

Electronic geometry: trigonal planar

Molecular geometry: trigonal planar

Bond angle: 120°



SHAPES OF MOLECULES

Compound: SO_2

Structure Type: AX_2E

3 groups

3 hybrid orbitals have formed

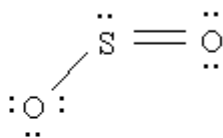
3 atomic orbitals were mixed

Hybridization: sp^2

Electronic geometry: trigonal planar

Molecular geometry: bent or angular

Bond angle: slightly $< 120^\circ$



Compound: CH_4

Structure Type: AX_4

4 groups

4 hybrid orbitals have formed

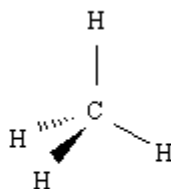
4 atomic orbitals were mixed

Hybridization: sp^3

Electronic geometry: tetrahedral

Molecular geometry: tetrahedral

Bond angle: 109.5°



Compound: NH_3

Structure Type: AX_3E

4 groups

4 hybrid orbitals have formed

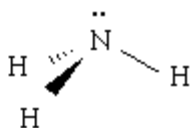
4 atomic orbitals were mixed

Hybridization: sp^3

Electronic geometry: tetrahedral

Molecular geometry: trigonal pyramidal

Bond angle: slightly $< 109.5^\circ$



Compound: H_2O

Structure Type: AX_2E_2

4 groups

4 hybrid orbitals have formed

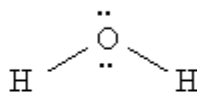
4 atomic orbitals were mixed

Hybridization: sp^3

Electronic geometry: tetrahedral

Molecular geometry: bent or angular

Bond angle: slightly $< 109.5^\circ$



SHAPES OF MOLECULES

Compound: PCl_5

Structure Type: AX_5

5 groups

5 hybrid orbitals have formed

5 atomic orbitals were mixed

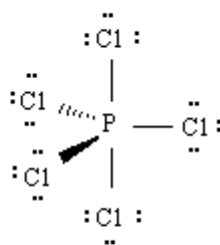
Hybridization: sp^3d

Electronic geometry: trigonal bipyramidal

Molecular geometry: trigonal bipyramidal

Bond angle: axial bonds are 180°

equatorial bonds are 120°



Compound: SF_4

Structure Type: AX_4E

5 groups

5 hybrid orbitals have formed

5 atomic orbitals were mixed

Hybridization: sp^3d

Electronic geometry: trigonal bipyramidal

Molecular geometry: seesaw

Bond angle: axial bonds are 180°

equatorial bonds are 120°



Compound: IBr_3

Structure Type: AX_3E_2

5 groups

5 hybrid orbitals have formed

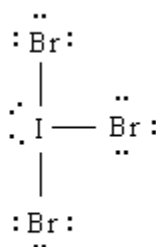
5 atomic orbitals were mixed

Hybridization: sp^3d

Electronic geometry: trigonal bipyramidal

Molecular geometry: T-shaped

Bond angle: slightly $< 90^\circ$



Compound: XeF_2

Structure Type: AX_2E_3

5 groups

5 hybrid orbitals have formed

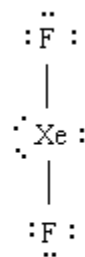
5 atomic orbitals were mixed

Hybridization: sp^3d

Electronic geometry: trigonal bipyramidal

Molecular geometry: linear

Bond angle: axial bonds are 180°



SHAPES OF MOLECULES

Compound: SF₆

Structure Type: AX₆

6 groups

6 hybrid orbitals have formed

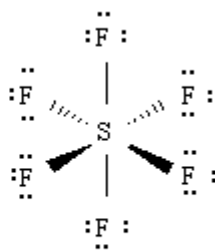
6 atomic orbitals were mixed

Hybridization: sp³d²

Electronic geometry: octahedral

Molecular geometry: octahedral

Bond angle: 90° and 180°



Compound: IF₅

Structure Type: AX₅E

6 groups

6 hybrid orbitals formed

6 atomic orbitals mixed

Hybridization: sp³d²

Electronic geometry: octahedral

Molecular geometry: square pyramidal

Bond angle: 90°



Compound: XeF₄

Structure Type: AX₄E₂

6 groups

6 hybrid orbitals have formed

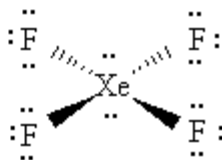
6 atomic orbitals were mixed

Hybridization: sp³d²

Electronic geometry: octahedral

Molecular geometry: square planar

Bond angle: 90°



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