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 \( \text{CO}_2 \)
Structure Type: \( AX_2 \)
2 groups
2 hybrid orbitals have formed
2 atomic orbitals were mixed
Hybridization: \( sp \)
Electronic geometry: linear
Molecular geometry: linear
Bond angle: 180°

Compound \( \text{H}_2\text{CO} \)
Structure Type: \( AX_3 \)
3 groups
3 hybrid orbitals have formed
3 atomic orbitals were mixed
Hybridization: \( sp^2 \)
Electronic geometry: trigonal planar
Molecular geometry: trigonal planar
Bond angle: 120°
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Compound: SO₂
Structure Type: AX₂E
3 groups
3 hybrid orbitals have formed
3 atomic orbitals were mixed
Hybridization: sp²
Electronic geometry: trigonal planar
Molecular geometry: bent or angular
Bond angle: slightly < 120°

Compound: CH₄
Structure Type: AX₄
4 groups
4 hybrid orbitals have formed
4 atomic orbitals were mixed
Hybridization: sp³
Electronic geometry: tetrahedral
Molecular geometry: tetrahedral
Bond angle: 109.5°

Compound: NH₃
Structure Type: AX₃E
4 groups
4 hybrid orbitals have formed
4 atomic orbitals were mixed
Hybridization: sp³
Electronic geometry: tetrahedral
Molecular geometry: trigonal pyramidal
Bond angle: slightly < 109.5°

Compound: H₂O
Structure Type: AX₂E₂
4 groups
4 hybrid orbitals have formed
4 atomic orbitals were mixed
Hybridization: sp³
Electronic geometry: tetrahedral
Molecular geometry: bent or angular
Bond angle: slightly < 109.5°
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Compound PCl₅
Structure Type: AX₅
5 groups
5 hybrid orbitals have formed
5 atomic orbitals were mixed
Hybridization: sp³d
Electronic geometry: trigonal bipyramidal
Molecular geometry: trigonal bipyramidal
Bond angle: axial bonds are 180°
equatorial bonds are 120°

Compound SF₄
Structure Type: AX₄E
5 groups
5 hybrid orbitals have formed
5 atomic orbitals were mixed
Hybridization: sp³d
Electronic geometry: trigonal bipyramidal
Molecular geometry: seesaw
Bond angle: axial bonds are 180°
equatorial bonds are 120°

Compound IBr₃
Structure Type: AX₃E₂
5 groups
5 hybrid orbitals have formed
5 atomic orbitals were mixed
Hybridization: sp³d
Electronic geometry: trigonal bipyramidal
Molecular geometry: T-shaped
Bond angle: slightly < 90°

Compound XeF₂
Structure Type: AX₂E₃
5 groups
5 hybrid orbitals have formed
5 atomic orbitals were mixed
Hybridization: sp³d
Electronic geometry: trigonal bipyramidal
Molecular geometry: linear
Bond angle: axial bonds are 180°
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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°