MOLECULAR GEOMETRY

VSEPR

• Valence Shell Electron Pair Repulsion theory.
• Most important factor in determining geometry is relative repulsion between electron pairs.

Lone Pair-Lone Pair < Lone Pair-Bond Pair < Bond pair-Bond pair repulsion

Geometries Predicted By The VSEPR
Molecular Structure Determination by VSEPR

Ammonia, NH₃
1. Draw electron dot structure

Structure Determination by VSEPR

Ammonia, NH₃
1. Draw electron dot structure
Structure Determination by VSEPR

Ammonia, NH₃

1. Draw electron dot structure

```
H—N—H
```

2. Count BP’s and LP’s around central N atom = 4

3. The 4 electron pairs are at the corners of a tetrahedron.

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Structure Determination by VSEPR

Ammonia, NH₃

1. Draw electron dot structure

```
H—N—H
```

2. Count BP’s and LP’s = 4

3. The 4 electron pairs are at the corners of a tetrahedron.

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Structure Determination by VSEPR

Ammonia, NH₃

1. Draw electron dot structure

```
H—N—H
```

2. Count BP’s and LP’s = 4

3. The 4 electron pairs are at the corners of a tetrahedron.

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lone pair of electrons in tetrahedral position
Structure Determination by VSEPR

Ammonia, NH₃

There are 4 electron pairs at the corners of a tetrahedron.

The ELECTRON PAIR GEOMETRY is tetrahedral.

The MOLECULAR GEOMETRY — the positions of the atoms — is PYRAMIDAL.

Water, H₂O

1. Draw electron dot structure
Structure Determination by VSEPR
Water, H₂O
1. Draw electron dot structure
   \[
   \begin{array}{c}
   H - O - H
   \end{array}
   \]
2. Count BP’s and LP’s = 4
3. The 4 electron pairs are at the corners of a tetrahedron.
   The electron pair geometry is TETRAHEDRAL.
Structure Determination by VSEPR

Water, H₂O

The electron pair geometry is TETRAHEDRAL.

The molecular geometry is bent.

Structure Determination by VSEPR

Formaldehyde, CH₂O

1. Draw electron dot structure

Structure Determination by VSEPR

Formaldehyde, CH₂O

1. Draw electron dot structure

H – C – H
Structure Determination by VSEPR

Formaldehyde, CH₂O

1. Draw electron dot structure
2. Count BP’s and LP’s = 3
   (the double bond is treated as a “lump” of electrons or one pair)

The electron pair geometry is PLANAR TRIGONAL with 120° bond angles.

The molecular geometry is also planar trigonal.
Structure Determination by VSEPR

Methanol, CH₃OH

1. Draw electron dot structure

2. Define bond angles 1 and 2

Angle 1 = 109°
Angle 2 = 105°

In both cases the atom is surrounded by 4 electron pairs.
Structure Determination by VSEPR

Acetonitrile, CH$_3$CN

Draw the electron dot structure

Define bond angles 1 and 2

Angle 1 = 109°
Angle 2 = 180°

One C is surrounded by 4 electron “lumps” and the other by 2 “lumps”
Phenylalanine, an amino acid

![Phenylalanine structure](image)

Phenylalanine

![Phenylalanine molecular structure](image)

STRUCTURES WITH CENTRAL ATOMS THAT DO NOT OBEY THE OCTET RULE

![Molecules with central atoms](image)
Violations of the Octet Rule

Usually occurs with Group 3A elements and with those of 3rd period and higher.
Consider boron trifluoride, BF\textsubscript{3}

Consider boron trifluoride, BF\textsubscript{3}
The B atom is surrounded by only 3 electron pairs.
Bond angles are 120°
Geometry described as planar trigonal
Compounds with 5 or 6 Pairs Around the Central Atom

- Trigonal bipyramid
  - 90° 120° 5 electron pairs

Compounds with 5 or More Pairs Around the Central Atom

- Trigonal bipyramid 90° 5 electron pairs
- Octahedron 6 electron pairs
**Sulfur Tetrafluoride, SF$_4$**

- Number of valence electrons = 34
- Central atom = S
- Dot structure

Electron pair geometry = ?
Sulfur Tetrafluoride, SF₄

- Number of valence electrons = 34
- Central atom = S
- Dot structure

Electron pair geometry = trigonal bipyramid (because there are 5 pairs around the S)

Lone pair is in the equator because it requires more room.

Multiple Bonds and Molecular Geometry

Lewis structure, one resonance structure, electron pair geometry = trigonal planar
Molecular structure, trigonal planar
Multiple Bonds and Molecular Geometry

Lewis structure, one resonance structure. Electron pair geometry = trigonal planar

Molecular structure, angular or bent

Multiple Bonds and Molecular Geometry

Electron pair geometry = trigonal planar