

## Objective

To construct different molecules and predict their molecular geometry using the VSEPR theory.

## Theory

Chemical bonding determines not only how atoms combine but also the shape of the molecules formed. The Lewis structure concept helps in understanding the arrangement of electrons but does not adequately explain molecular shapes. To overcome this limitation, the Valence Shell Electron Pair Repulsion (VSEPR) Theory was proposed by Sidgwick and Powell (1940) and later refined by Nyholm and Gillespie (1957).

According to VSEPR theory, the shape of a molecule depends upon the number of electron pairs present around the central atom. These electron pairs may be bonding pairs or lone pairs. Since electron pairs are negatively charged, they repel each other and arrange themselves in such a way that repulsion is minimized and the distance between them is maximized.

The main postulates of VSEPR theory are:

- The shape of a molecule depends on the number of valence shell electron pairs around the central atom.
- Electron pairs repel one another due to their negative charge.
- Electron pairs occupy positions that minimize repulsion and maximize separation.
- Multiple bonds are treated as a single region of electron density.
- The theory can be applied to molecules represented by resonance structures.

The repulsive interactions decrease in the following order:

**Lone Pair–Lone Pair > Lone Pair–Bond Pair > Bond Pair–Bond Pair**

Since lone pairs occupy more space than bonding pairs, they exert greater repulsion, resulting in deviations from ideal bond angles and molecular geometries.

For molecules without lone pairs on the central atom, the geometry depends on the number of bonded atoms:

| Type of Molecule | Example          | Dipole Moment, $\mu$ (D) | Geometry           |
|------------------|------------------|--------------------------|--------------------|
| AB               | HF               | 1.78                     | Linear             |
| AB               | HCl              | 1.07                     | Linear             |
| AB               | HBr              | 0.79                     | Linear             |
| AB               | HI               | 0.38                     | Linear             |
| AB               | H <sub>2</sub>   | 0.00                     | Linear             |
| AB <sub>2</sub>  | H <sub>2</sub> O | 1.85                     | Bent               |
| AB <sub>2</sub>  | H <sub>2</sub> S | 0.95                     | Bent               |
| AB <sub>2</sub>  | CO <sub>2</sub>  | 0.00                     | Linear             |
| AB <sub>3</sub>  | NH <sub>3</sub>  | 1.47                     | Trigonal Pyramidal |
| AB <sub>3</sub>  | NF <sub>3</sub>  | 0.23                     | Trigonal Pyramidal |

|                 |                   |      |                 |
|-----------------|-------------------|------|-----------------|
| AB <sub>3</sub> | BF <sub>3</sub>   | 0.00 | Trigonal Planar |
| AB <sub>4</sub> | CH <sub>4</sub>   | 0.00 | Tetrahedral     |
| AB <sub>4</sub> | CHCl <sub>3</sub> | 1.04 | Tetrahedral     |
| AB <sub>4</sub> | CCl <sub>4</sub>  | 0.00 | Tetrahedral     |

VSEPR theory successfully predicts the geometry of a large number of covalent molecules and ions, particularly those formed by p-block elements.

### Learning Outcomes

1. Construct molecular models and identify their molecular formulae using a virtual simulator.
2. Apply VSEPR theory to predict the geometry of simple covalent molecules.
3. Classify molecules as linear, bent, trigonal planar, trigonal pyramidal, or tetrahedral based on electron pair arrangement.
4. Relate molecular shape and symmetry to the dipole moment of a molecule.
5. Compare observed molecular geometries with theoretical predictions of VSEPR theory.