

SHAPES OF MOLECULES

The shapes of molecules can be described and predicted using a simple model based largely on Lewis structures.

Valence shell electron pair repulsion (VSEPR) theory states that the electron pairs surrounding an atom tend to repel each other.

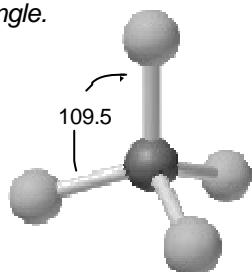
The best arrangement of a given number of electron domains is the one that minimizes the repulsions among them.

Electron-domain geometry indicates the arrangement of electron pairs about the central atom AB_n .

Number of Electron Domains	Arrangement of Electron Domains	Electron-Domain Geometry	Typical Bond Angle
2		Linear	180°
3		Trigonal planar	120°
4		Tetrahedral	109.5°
5		Trigonal bipyramidal	120° 90°
6		Octahedral	90° 180°

Molecular geometry of a molecule (or ion) indicates the arrangement of atoms in space about the central atom.

The angle formed by any two atoms bonded to the central atom is referred to as the *bond angle*.



Summary of VSEPR Geometries

Bonding Domains	Nonbonding Domains	e ⁻ domain Geometry	Molecular Shape	Bond Angle
4	0	tetrahedral	tetrahedral	109.5°
3	0	equilateral triangle planer	triangular	120°
3	1	tetrahedral	triangular pyramidal	107°
2	2	tetrahedral	angular	104.5°
2	0	linear	linear	180°
1	3	tetrahedral	linear	----
2	1	equilateral triangle	bent	----

MOLECULES WITH EXPANDED VALENCE SHELLS

Bonding Domains	Nonbonding Domains	Molecular Geometry
5	0	Trigonal bipyramidal
4	1	Seesaw
3	2	T-shaped
2	3	Linear
6	0	Octahedral
5	1	Square pyramidal
4	2	Square planar

TABLE 9.2 Electron Domain Geometries and Molecular Shapes for Molecules with Two, Three, and Four Electron Domains About the Central Atom

Total Electron Domains	Electron Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
2 domains	Linear	2	0	Linear	CO ₂
3 domains	Trigonal planar	3	0	Trigonal planar	BF ₃
		2	1	Bent	SO ₂
4 domains	Tetrahedral	4	0	Tetrahedral	CH ₄
		3	1	Trigonal pyramidal	NH ₃
		2	2	Bent	H ₂ O

TABLE 9.3 Electron Domain Geometries and Molecular Shapes for Molecules with Five and Six Electron Domains About the Central Atom

Total Electron Domains	Electron Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
5 domains	Trigonal bipyramidal	5	0	Trigonal bipyramidal	PCl ₅
		4	1	Seesaw	SF ₄
		3	2	T-shaped	ClF ₃
		2	3	Linear	XeF ₂
6 domains	Octahedral	6	0	Octahedral	SF ₆
		5	1	Square pyramidal	BrF ₅
		4	2	Square planar	BrF ₄ ²⁻

In terms of the volume occupied by electron domains:

lone pairs > triple bonds > double bonds > single bonds