Nyholm and Gillespies's
Valence Shell Electron Pair Repulsion Theory
(V.S.E.P.R. Theory)
or
Electron Domain Theory[1]
(E.D. Theory)

L Electrons in bonded atoms occupy spatially oriented orbitals in such a way as to minimize electron-electron repulsions arising mainly from electrostatic (coulombic) forces.

- For every number of electron pairs about a central atom (2, 3, 4, 5, 6), there is a preferred arrangement that minimizes repulsions.

- The shape of a molecule is based on the preferred arrangement of electron pairs.

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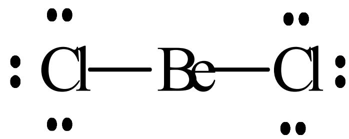
[1] R. J. Gillespie. *J. Chem. Educ.* **1992,** *69*, 116.

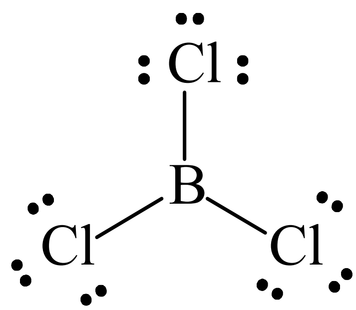
Basic Geometries for 2, 3, and 4 Electron Pairs

$BeCl_2$



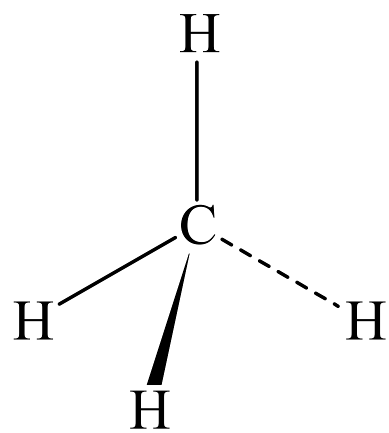
Two pairs minimize repulsions if oriented 180° from one another, giving a **linear** geometry.

BCl_3



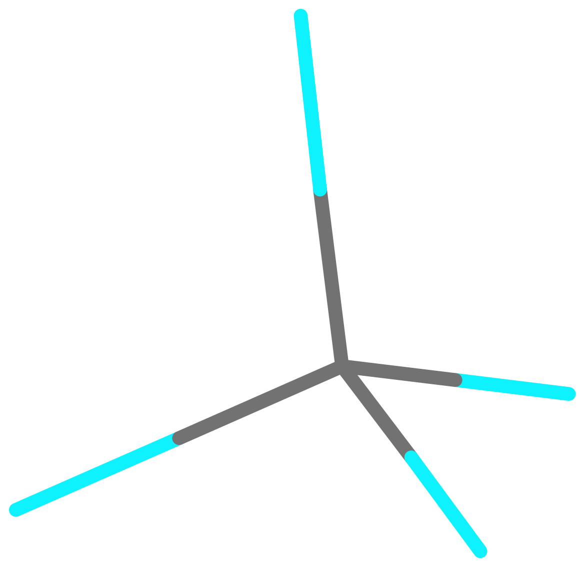
Three pairs minimize repulsions if oriented 120° from one another, giving a **trigonal planar** geometry.

CH_4

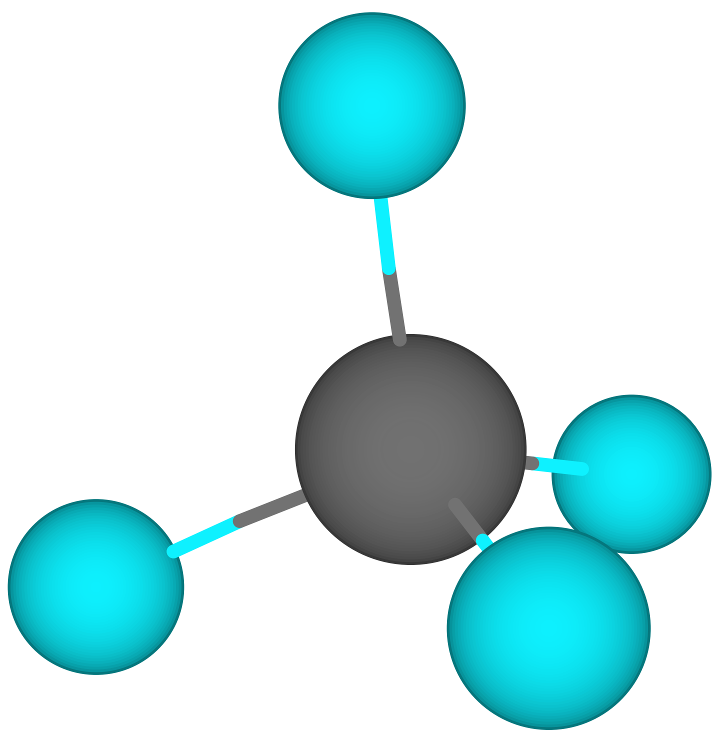


Four pairs minimize repulsions if oriented 109.5° from one another, giving a **tetrahedral** geometry.

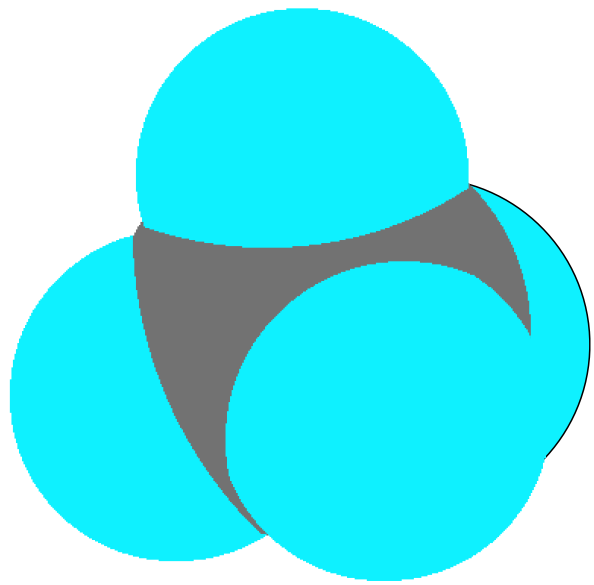
Stick Model of CH_4



Ball-and-Stick Model of CH_4



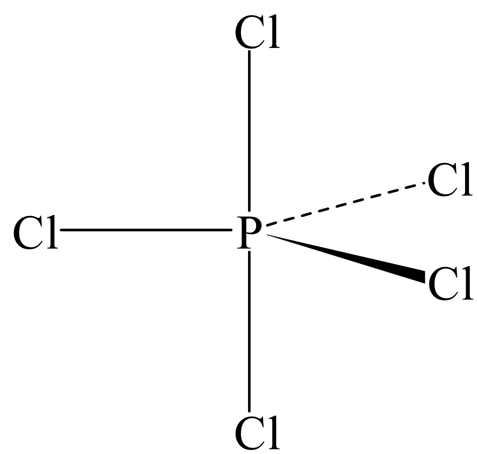
Space-Filling Model of CH_4



Basic Geometry for 5 Electron Pairs

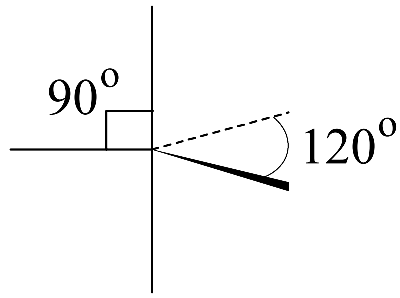
PCl_5

Five pairs minimize repulsions in a **trigonal bipyramidal** geometry.

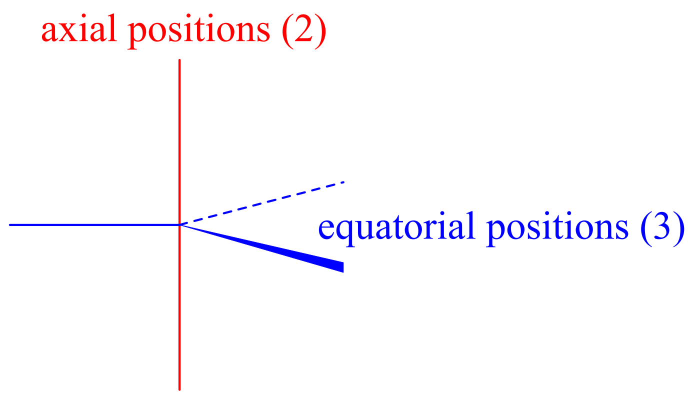


Geometry of a Trigonal Bipyramid (*tbp*)

Two angles:



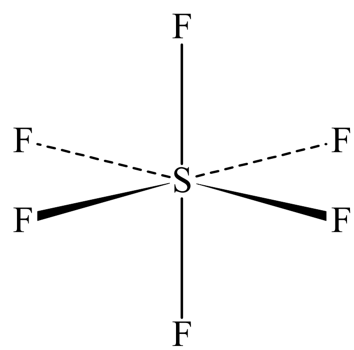
Two different kinds of positions:

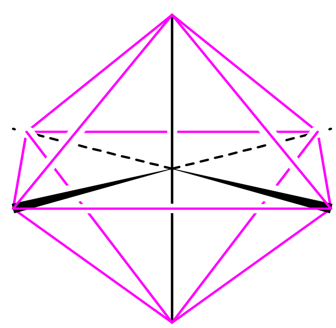


Basic Geometry for 6 Electron Pairs

SF_6

Six pairs minimize repulsions in an **octahedral** geometry.

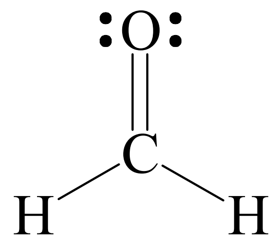




All positions are equivalent and form 90^{o} or 180^{o} angles to each other.

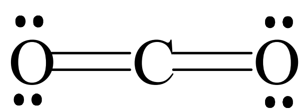
Molecules with Double Bonds

L Shape is determined by the number of *electron domains* (regions), not simply the number of electron pairs.



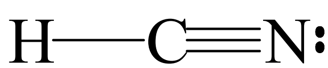
4 pairs in 3 regions

Y trigonal planar



4 pairs in 2 regions

Y linear

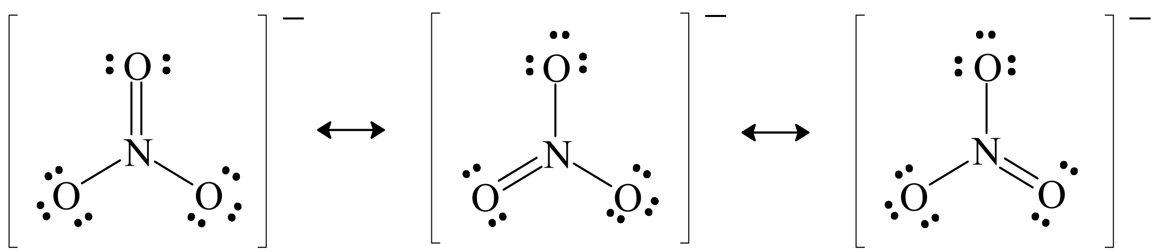


4 pairs in 2 regions

Y linear

Resonance Hybrid Molecules

L Any individual resonance (canonical) form can be used to predict the shape, treating "multiple bonds" as if they were real.



4 pairs in 3 regions in any canonical form

Y trigonal planar

Molecules with Lone Pairs (Non-Bonding Pairs) On the Central Atom

1. Shape refers to the geometrical arrangement of the atoms relative to one another in a molecule, *not* to the idealized arrangement of electron domains.

2. Molecules with non-bonding pairs on a central atom have shapes based on the arrangement of the electron domains, but bond angles may be slightly altered by repulsions among lone pairs (l.p.) and bond pairs (b.p.), which diminish in strength in the order

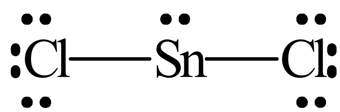
   l.p.-l.p. > l.p.-b.p. > b.p.-b.p.

3. Shapes of molecules based on a *tbp* geometry of electron domains (5 pairs) result from preferentially placing any lone pairs in equatorial positions.

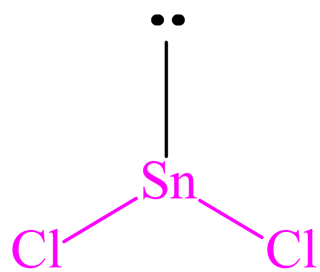
Three Electron Domains
2 b.p + 1 l.p.

$SnCl_2$

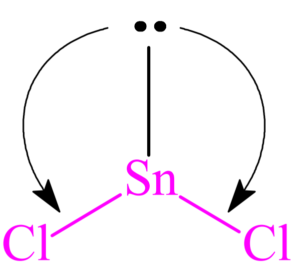
Lewis model:



Shape: **Bent**



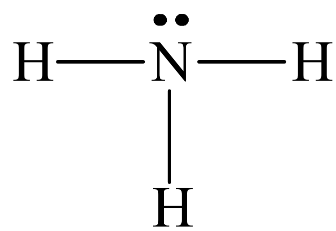
L.p.-b.p. repulsions cause the Cl-Sn-Cl angle to close to less than 120^{o}.



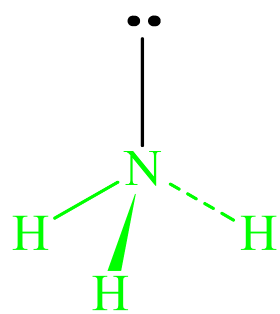
Four Electron Domains
3 b.p. + 1 l.p.

NH_3

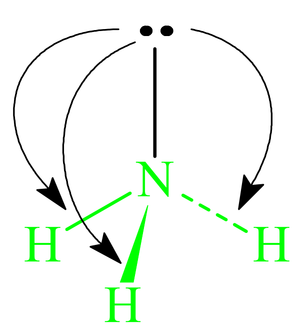
Lewis model:



Shape: **Trigonal Pyramid**



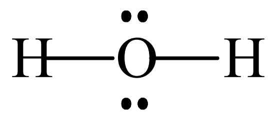
L.p.-b.p. repulsions cause the H-N-H angles to close to less than 109.5^{o} (~107^{o}).



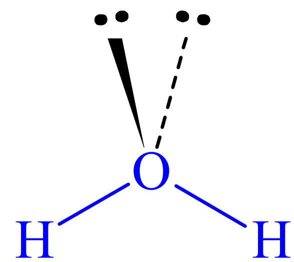
Four Electron Domains
2 b.p. + 2 l.p.

H_2O

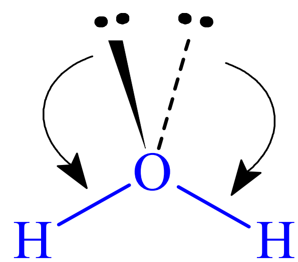
Lewis model:



Shape: **Bent**



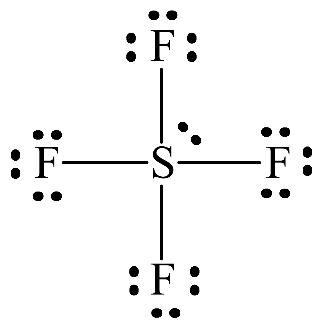
L.p.-b.p. repulsions cause the H-O-H angle to close to less than 109.5 ^{o} (104.5 ^{o}).



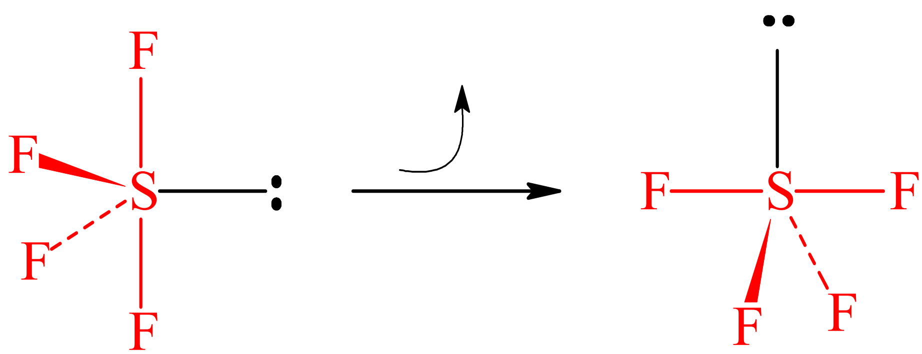
Five Electron Domains
4 b.p. + 1 l.p.

SF_4

Lewis model:



Shape: **Irregular Tetrahedron ("see-saw" shape)**



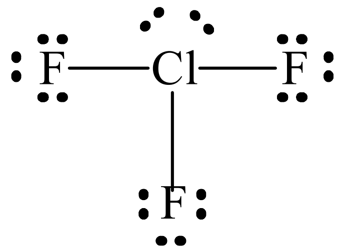
Note: Lone pair occupies an equatorial position of *tbp*.

L.p.-b.p. repulsions cause both F-S-F angles to close to less than 120^{o} and 180^{o}, respectively.

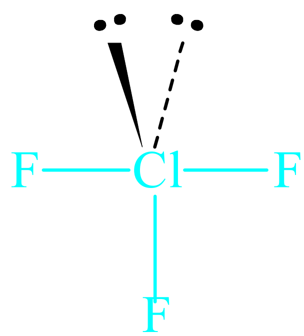
Five Electron Domains
3 b.p. + 2 l.p.

ClF_3

Lewis model:



Shape: **T-shape**



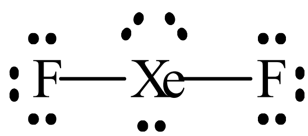
Note: Lone pairs occupy equatorial positions of *tbp*.

L.p.-b.p. repulsions cause both F-Cl-F angles to close to less than 90°.

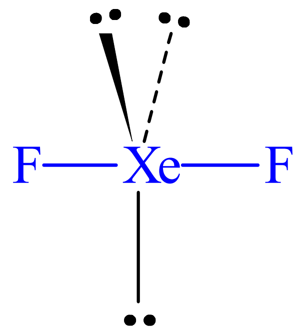
Five Electron Domains
2 b.p. + 3 l.p.

XeF_2

Lewis model:



Shape: **Linear**



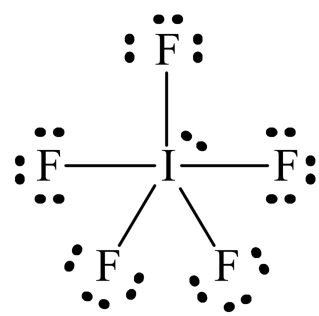
Note: Lone pairs occupy equatorial positions of *tbp*.

L.p.-b.p. repulsions *do not* cause angle distortions in this case, but rather enforce the linearity of the molecule.

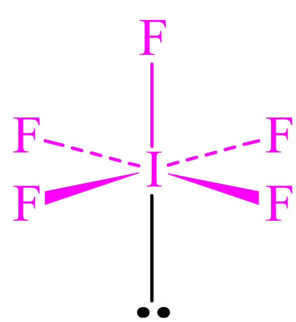
Six Electron Domains
5 b.p. + 1 l.p.

IF_5

Lewis Model:



Shape: **Square Pyramid**

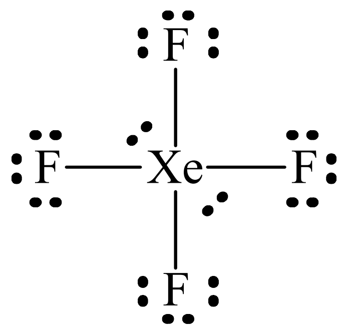


L.p.-b.p. repulsions cause the plane of the four basal F atoms to move slightly above the I atom, making the F-I-F angle between any basal F and the axial F less than 90^{o}.

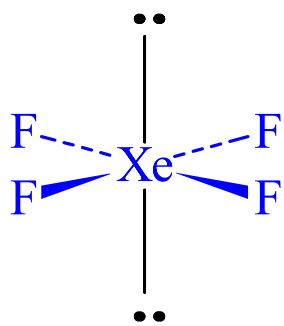
Six Electron Domains
4 b.p. + 2 l.p.

XeF_4

Lewis model:



Shape: **Square Planar**



Note: Lone pairs occupy opposite positions to minimize l.p.-l.p repulsions.

L.p.-b.p. repulsions *do not* cause angle distortions in this case, but rather enforce the planarity of the molecule.

SHAPES OF MX_n MOLECULES BY V.S.E.P.R. THEORY

Electron Regions	Arrangement of Regions	Bond Domains[2]	Lone Pairs	Molecular Shape	Polar?[3]
2	linear	2	0	linear [MX_2]	No
3	trigonal planar	3	0	trigonal planar [MX_3]	No
		2	1	bent (<120°) [MX_2]	Yes
4	tetrahedral	4	0	tetrahedral [MX_4]	No
		3	1	trigonal pyramidal [MX_3]	Yes
		2	2	bent (<109.5°) [MX_2]	Yes
5	trigonal bipyramidal	5	0	trigonal bipyramidal [MX_5]	No
		4	1	irregular tetrahedron [MX_4]	Yes
		3	2	T-shaped [MX_3]	Yes
		2	3	linear [MX_2]	No
6	octahedral	6	0	octahedral [MX_6]	No
		5	1	square pyramid [MX_5]	Yes
		4	2	square planar [MX_4]	No

[2]A single, double, or triple bond constitutes one domain of electron density. Therefore, count bond domains around the central atom (i.e., the number of atom-pair linkages), not numbers of electron pairs. For this reason, the co-author of V.S.E.P.R. theory has renamed it the Electron Domain theory. [R. J. Gillespie. *J. Chem. Educ.* **1992,** *69*, 116.]

[3]Listed polarity is for *binary* compounds (MX_n) only. Composition of ternary (MX_nY_m) and higher compounds may result in polarity for a shape that might be nonpolar if the compound were binary.

VSEPR-Predicted Shapes for MX_n Molecules (n = 2, 3, 4, 5, 6)

Formula	Case	Shape	Example
MX_2	2 bonds + 0 lone pairs	linear	BeF_2
	2 bonds + 1 lone pair	bent (<120°)	$SnCl_2$
	2 bonds + 2 lone pairs	bent (<109.5°)	H_2O
	2 bonds + 3 lone pairs	linear	XeF_2
MX_3	3 bonds + 0 lone pairs	trigonal planar	BF_3
	3 bonds + 1 lone pair	trigonal pyramidal	NH_3
	3 bonds + 2 lone pairs	T-shape	ClF_3
MX_4	4 bonds + 0 lone pairs	tetrahedral	CH_4
	4 bonds + 1 lone pair	irregular tetrahedron	SF_4
	4 bonds + 2 lone pairs	square planar	XeF_4
MX_5	5 bonds + 0 lone pairs	trigonal bipyramid (*tbp*)	PF_5
	5 bonds + 1 lone pair	square pyramid	IF_5
MX_6	6 bonds + 0 lone pairs	octahedral	SF_6

Note: In this table, “bond” means a linkage between two atoms in a molecule. Thus a single-, double-, or triple-bond constitutes only one bond.

Relationship Between Lewis Structures
and
Actual Molecular Geometry

L Lewis structures are inherently two dimensional and do not attempt to represent the true three-dimensional shape and angular relationships that exist in the actual molecule.

L V.S.E.P.R. theory can be used to estimate the actual bond angles in a molecule from the Lewis structure and the number of electron domains about each atom.