VSEPR Theory

(HS second year)

By Dr. Manash Jyoti Deka

Covalent Bond Theories

1. VSEPR (valence shell electron pair repulsion model).
   A set of *empirical* rules for predicting a molecular geometry using, as input, a correct Lewis Dot representation.

2. Valence Bond theory.
   A more advanced description of orbitals in molecules. We emphasize just one aspect of this theory: Hybrid atomic orbitals.
   Works especially well for organic molecules, which is the reason we don't scrap it entirely for MO theory.

3. Molecular Orbital theory.
   The most modern and powerful theory of bonding. Based upon QM.

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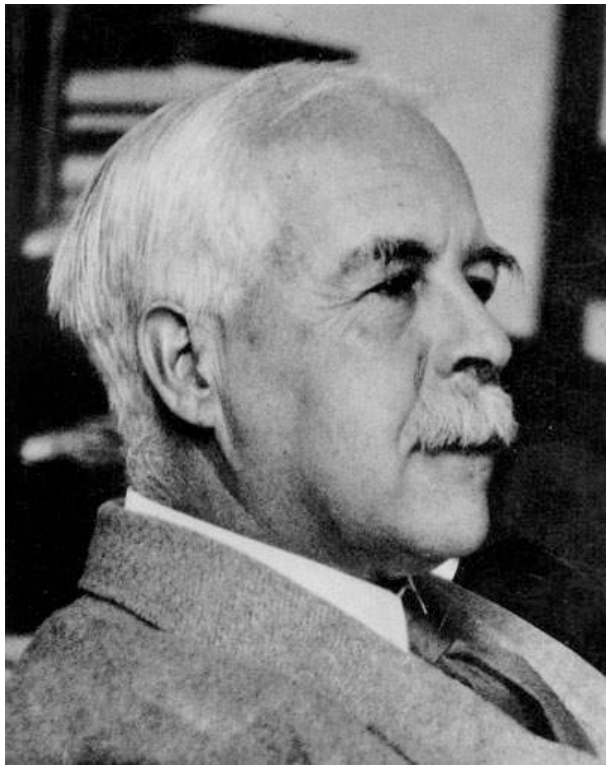
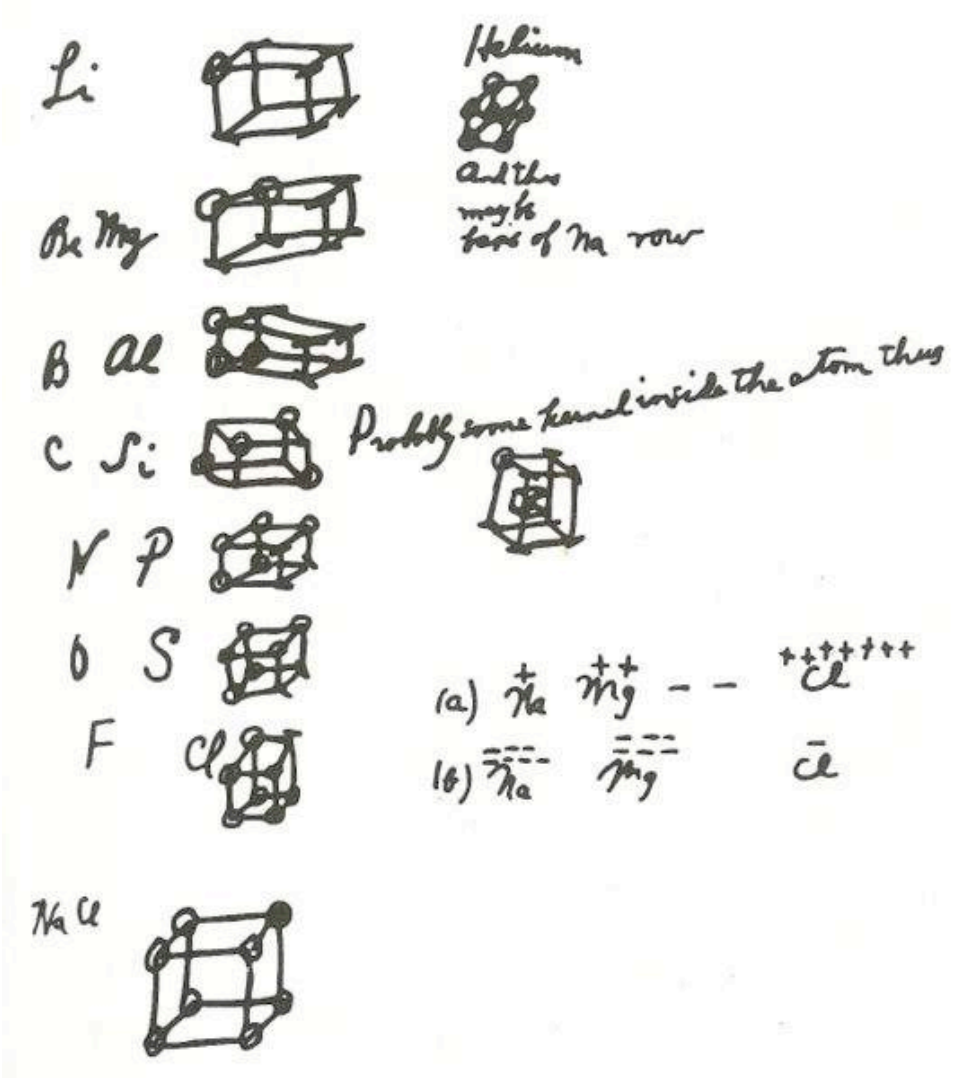
G. N. Lewis tried to develop a geometrical model for atoms and chemical bonding -- but failed.



G. N. Lewis
1875-1946



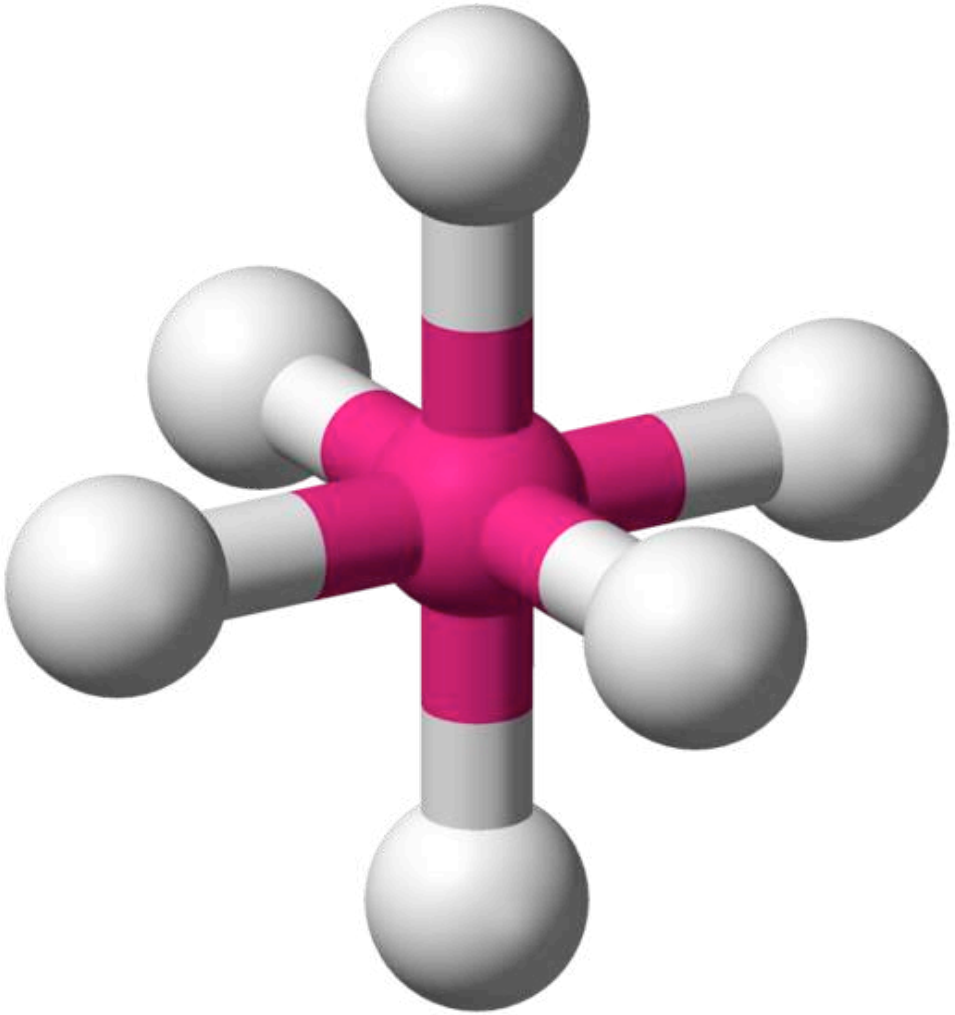
Gillespie and Nyholm devised a simple scheme for geometry based on the Lewis dot structure (VSEPR).

Valence shell electron pair repulsion (VSEPR) theory is a model in chemistry used to predict the shape of individual molecules based upon the extent of electron-pair electrostatic repulsion. It is also named Gillespie-Nyholm* theory after its two main developers. The acronym "VSEPR" is pronounced "vesper" for ease of pronunciation.

Ronald J. Gillespie
1924 -

*Ronald J. Gillespie and Ronald S. Nyholm
University College, London, 1957.

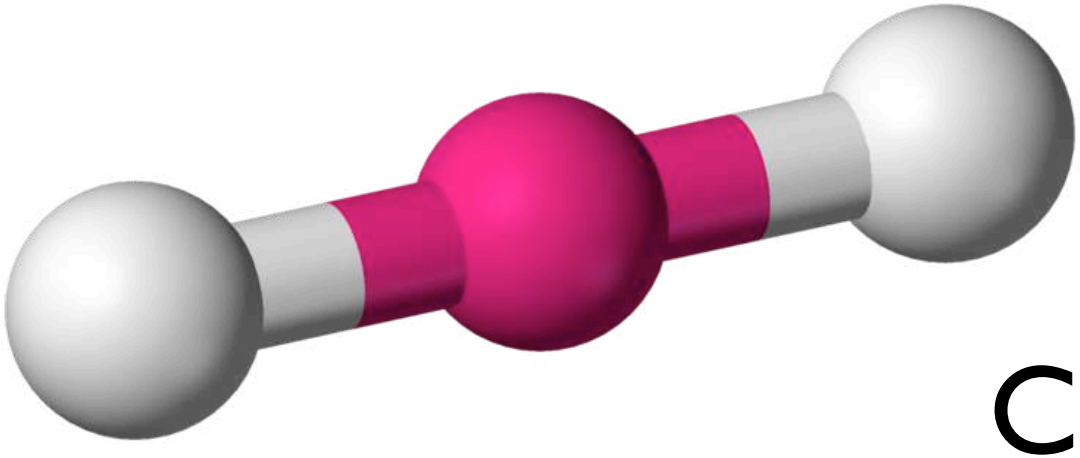
Living in 3 Dimensions



What role does geometry play in chemical structure?

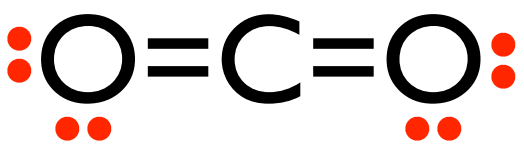
Gillespie and Nyholm looked at the structures of molecules of the form AX_n:

AX_2



CO_2

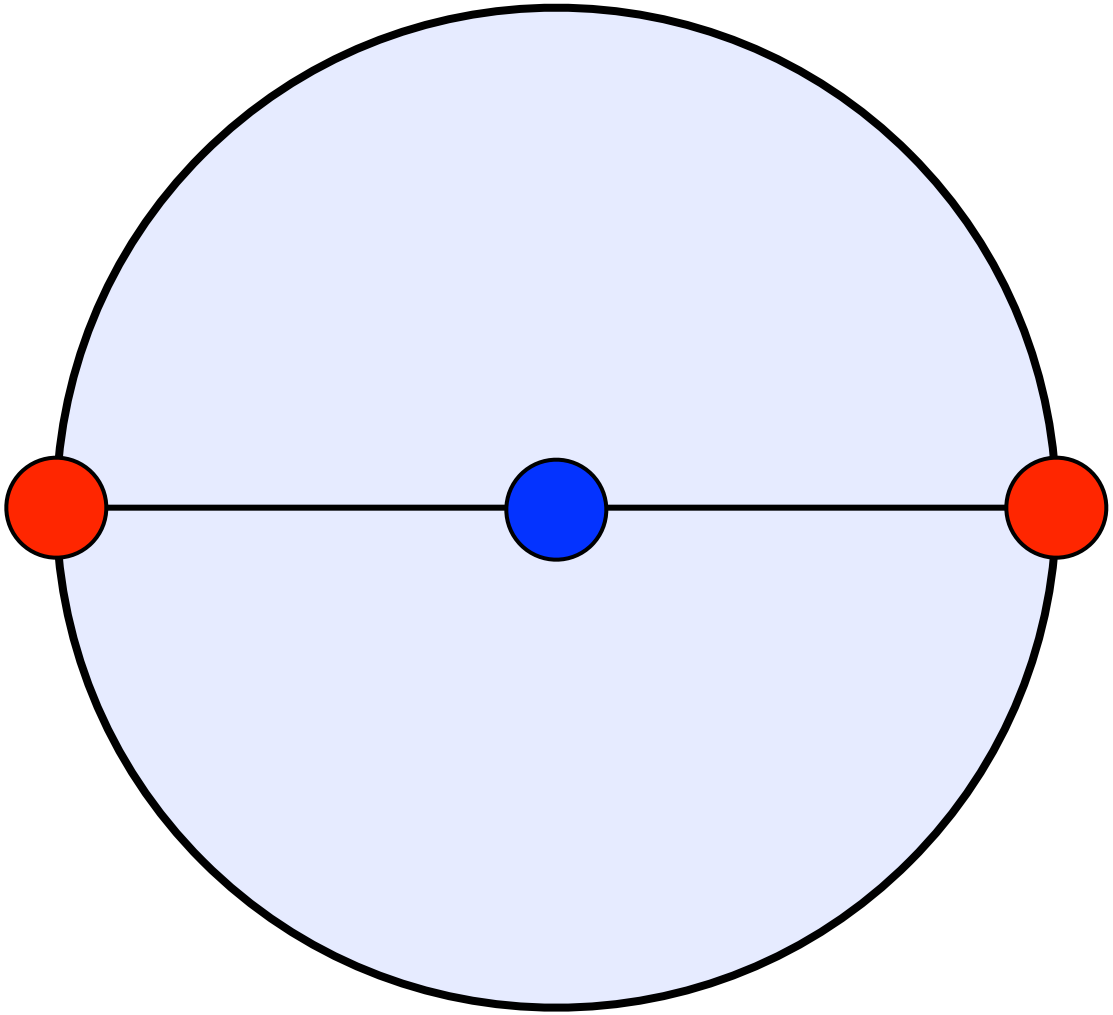
16 electrons



O-C-O angle: 180°

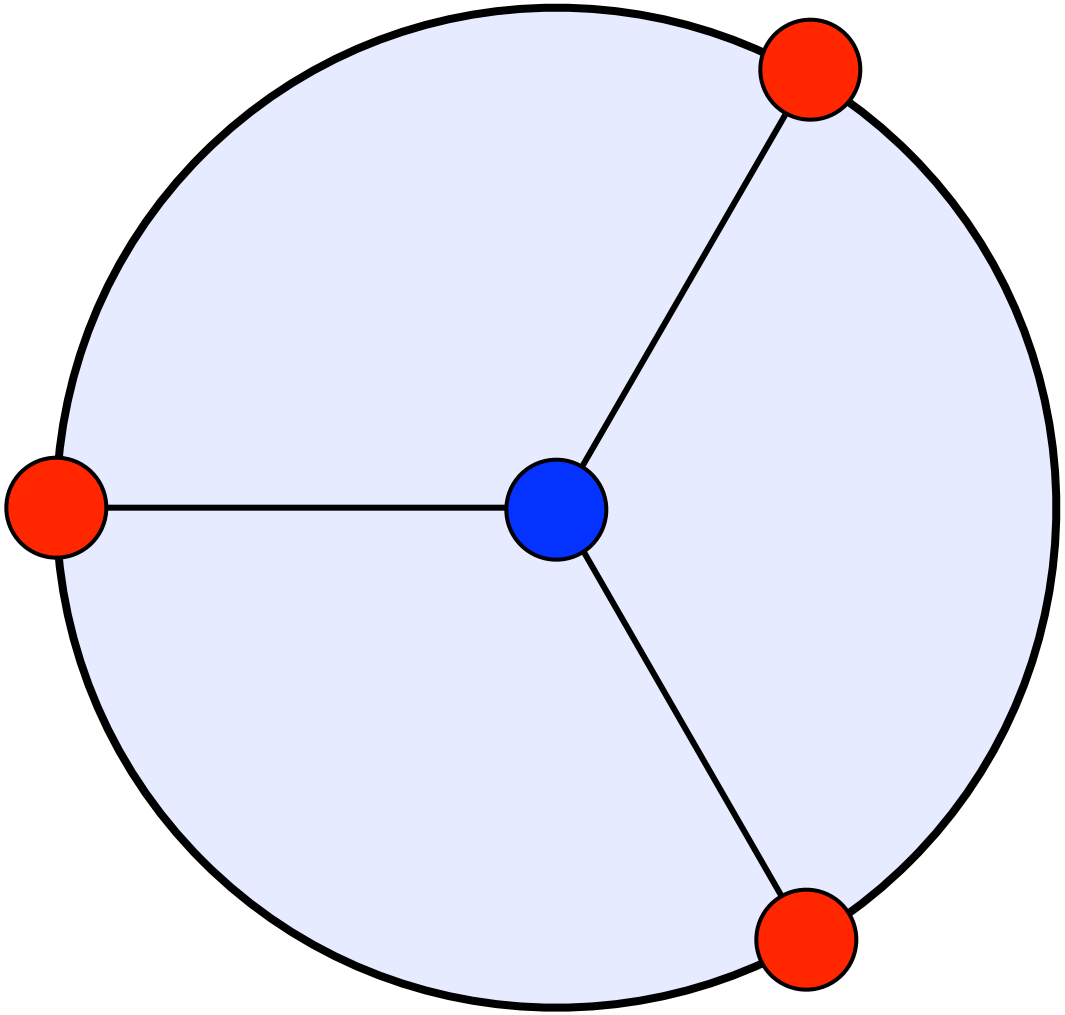
Linear Geometry

AX_2



X-A-X angle: 180°

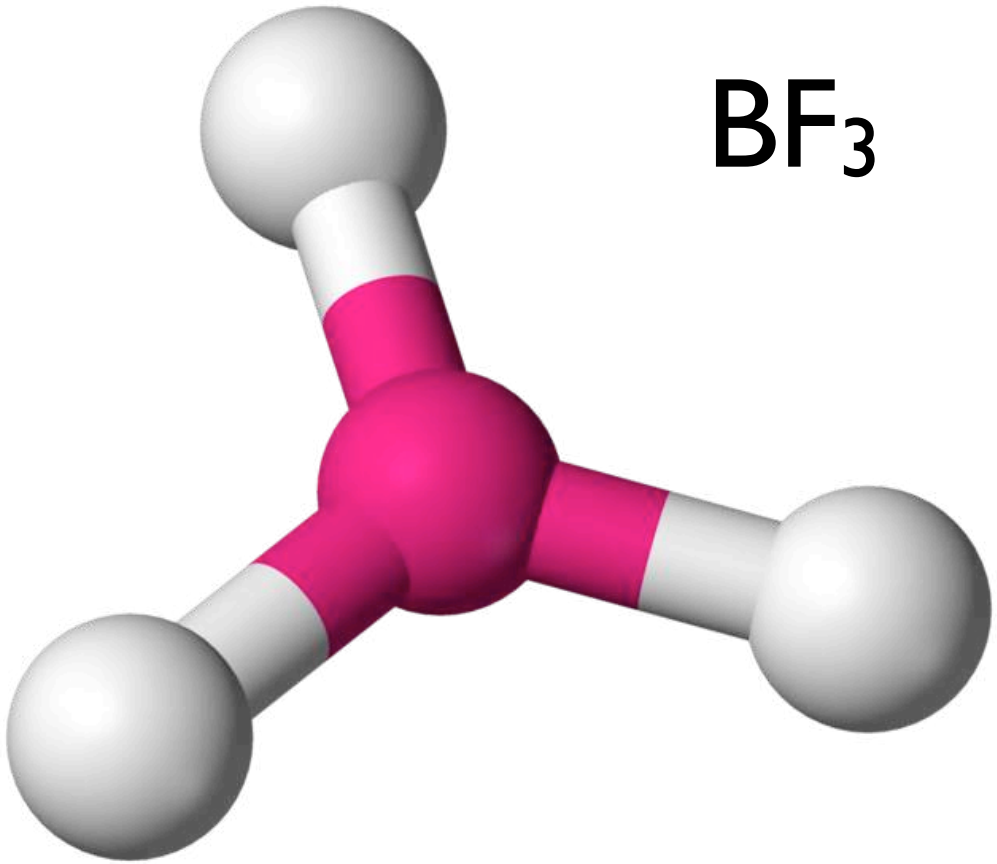
Linear Geometry



AX_3

X-A-X angle: 120°

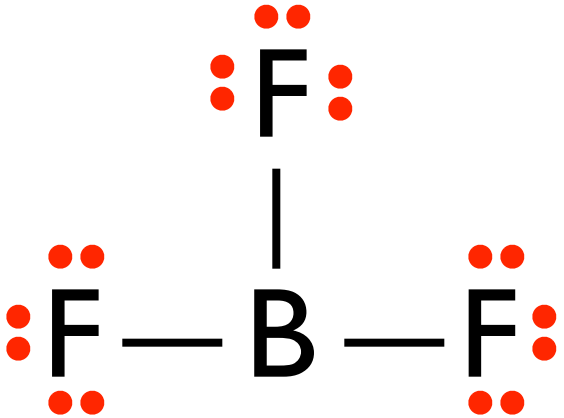
Trigonal Geometry



BF_3

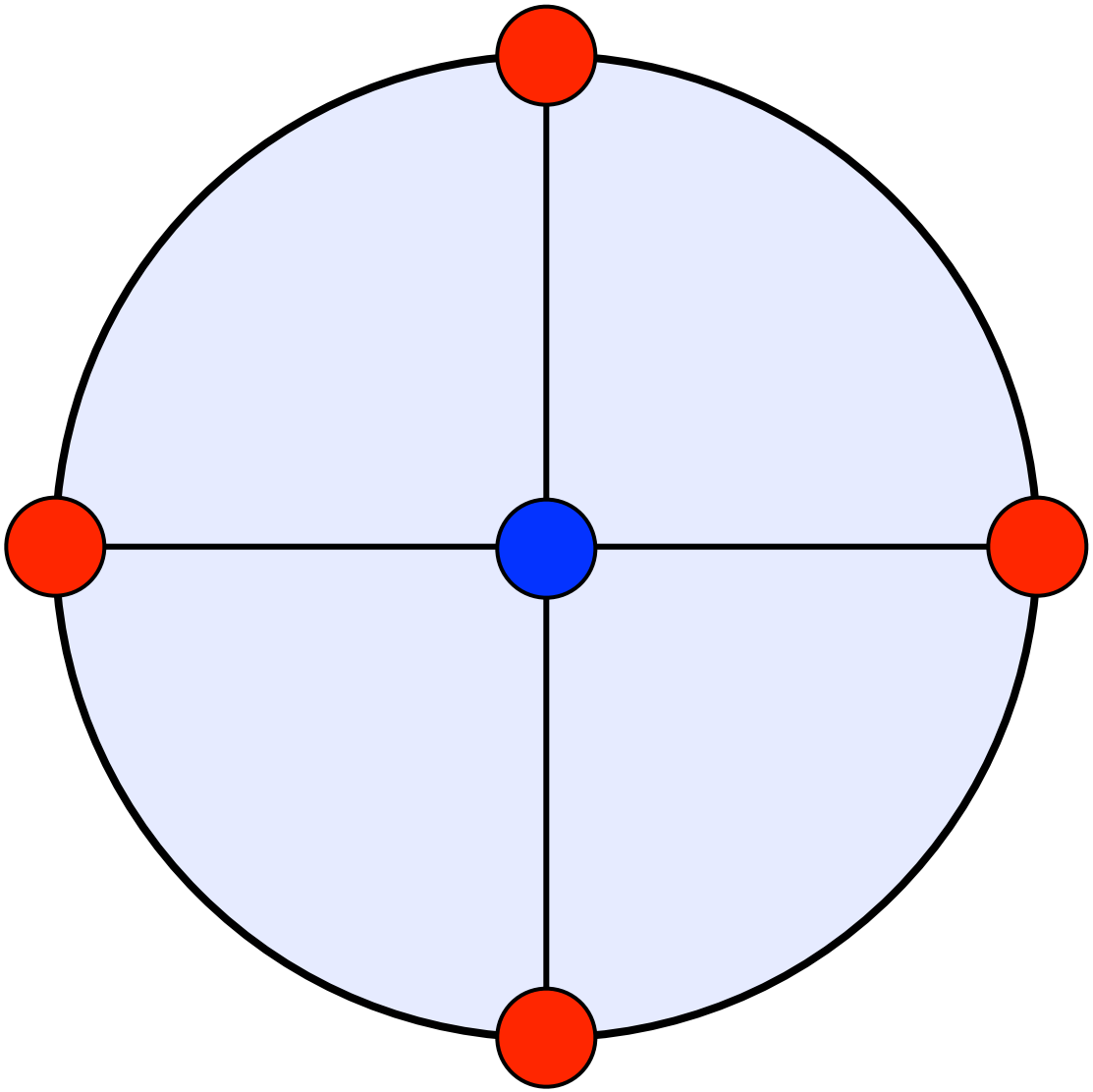
AX_3

24 electrons



F-B-F angle: 120°

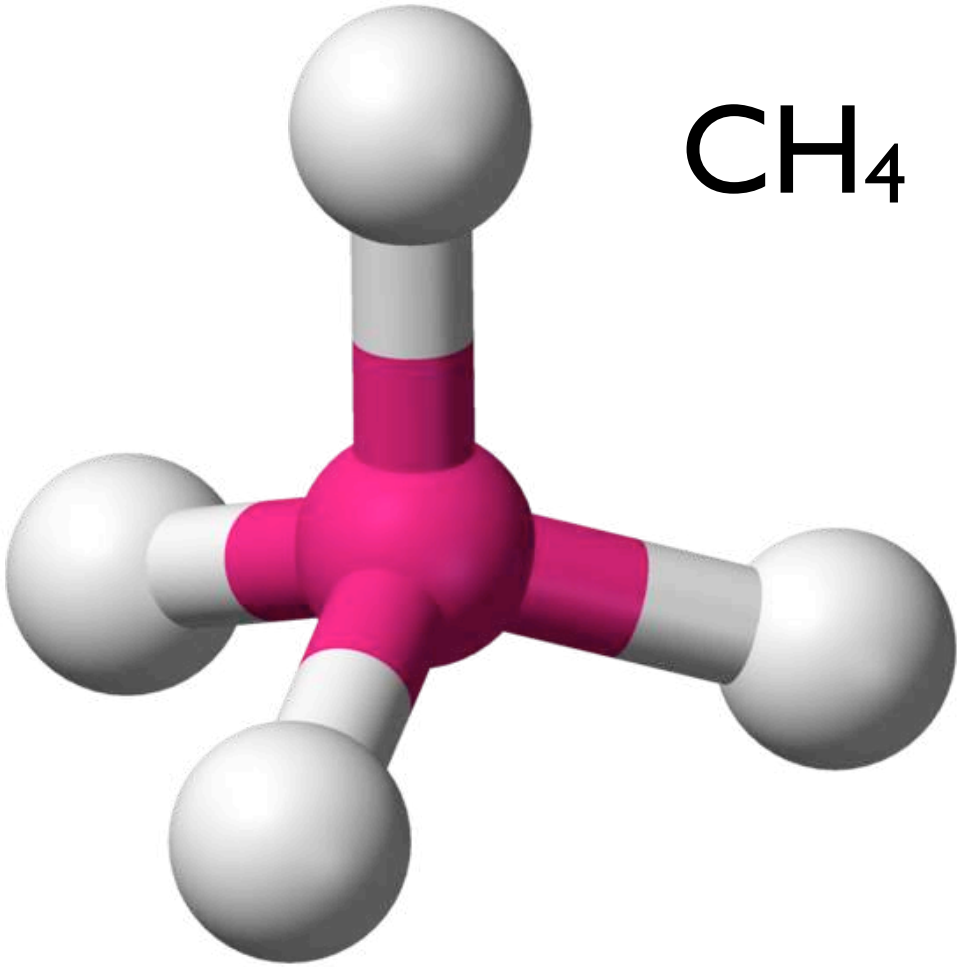
Trigonal Planar Geometry



AX_4

X-A-X angle: 90°

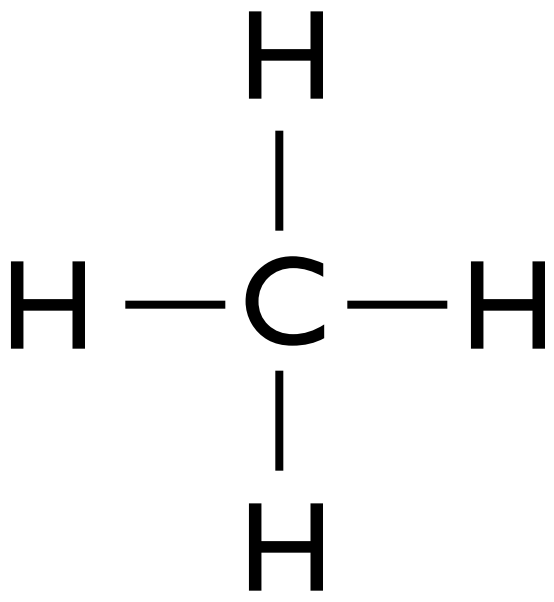
Square Planar Geometry?



CH_4

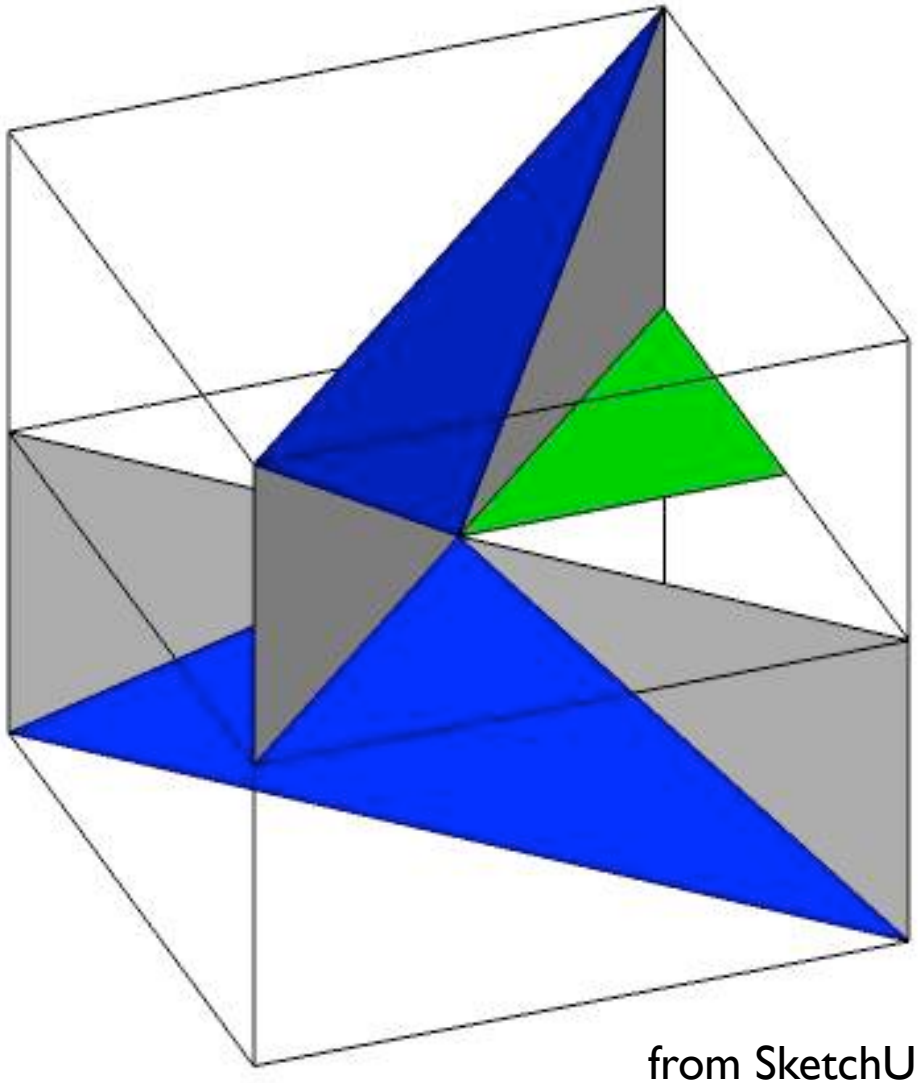
AX_4

8 electrons



H-C-H angle: ?

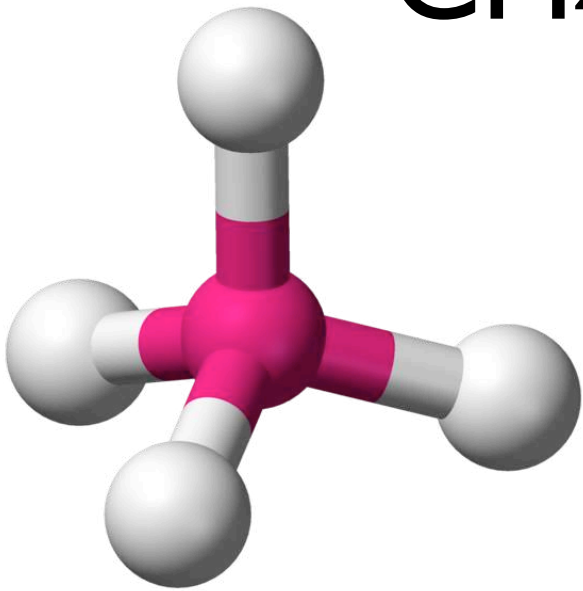
Tetrahedral Geometry



from SketchUp

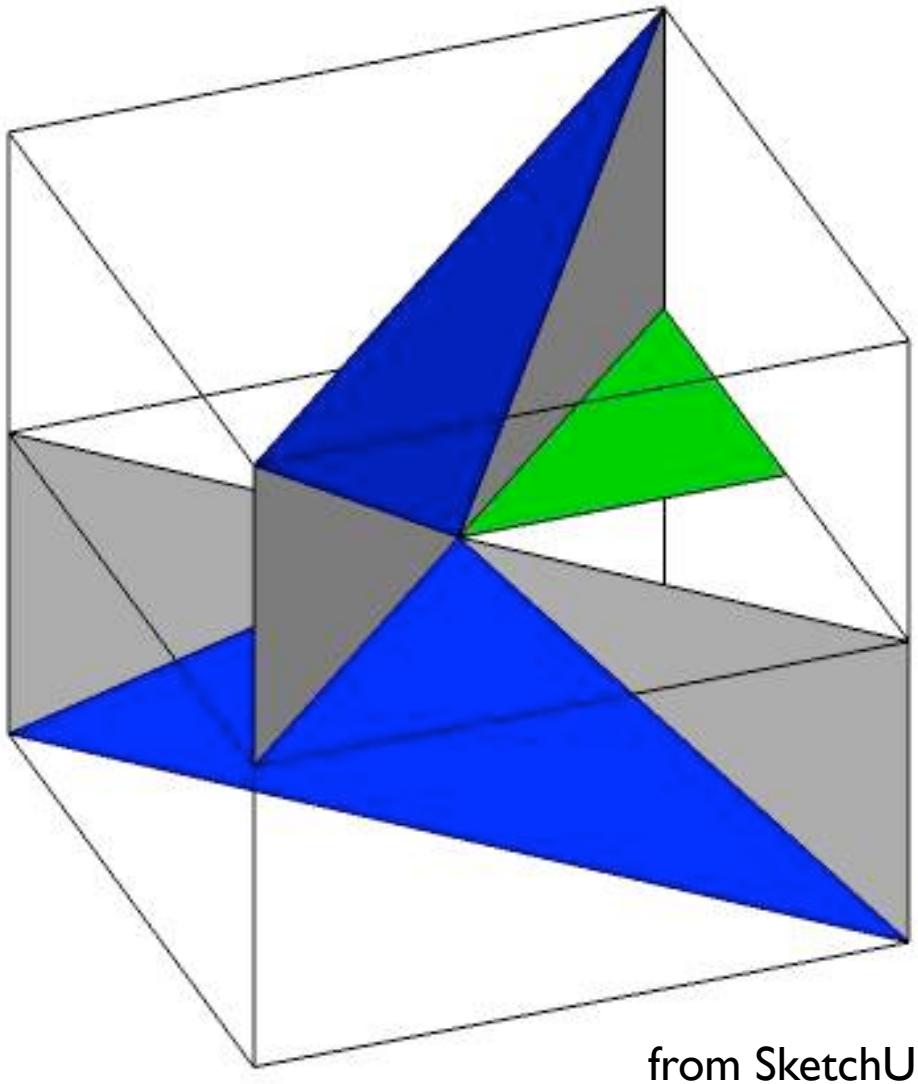
AX_4

CH_4



H-C-H angle: 109.47°

Tetrahedral Geometry



from SketchUp

AX_4

Green Triangle:

1 + 1 = 2

Hypotenuse = $\sqrt{2}$

Gray Triangle:

2 + 1 = 3

Hypotenuse = $\sqrt{3}$

Grey Angle = $\cos^{-1}(\sqrt{2}/\sqrt{3})$

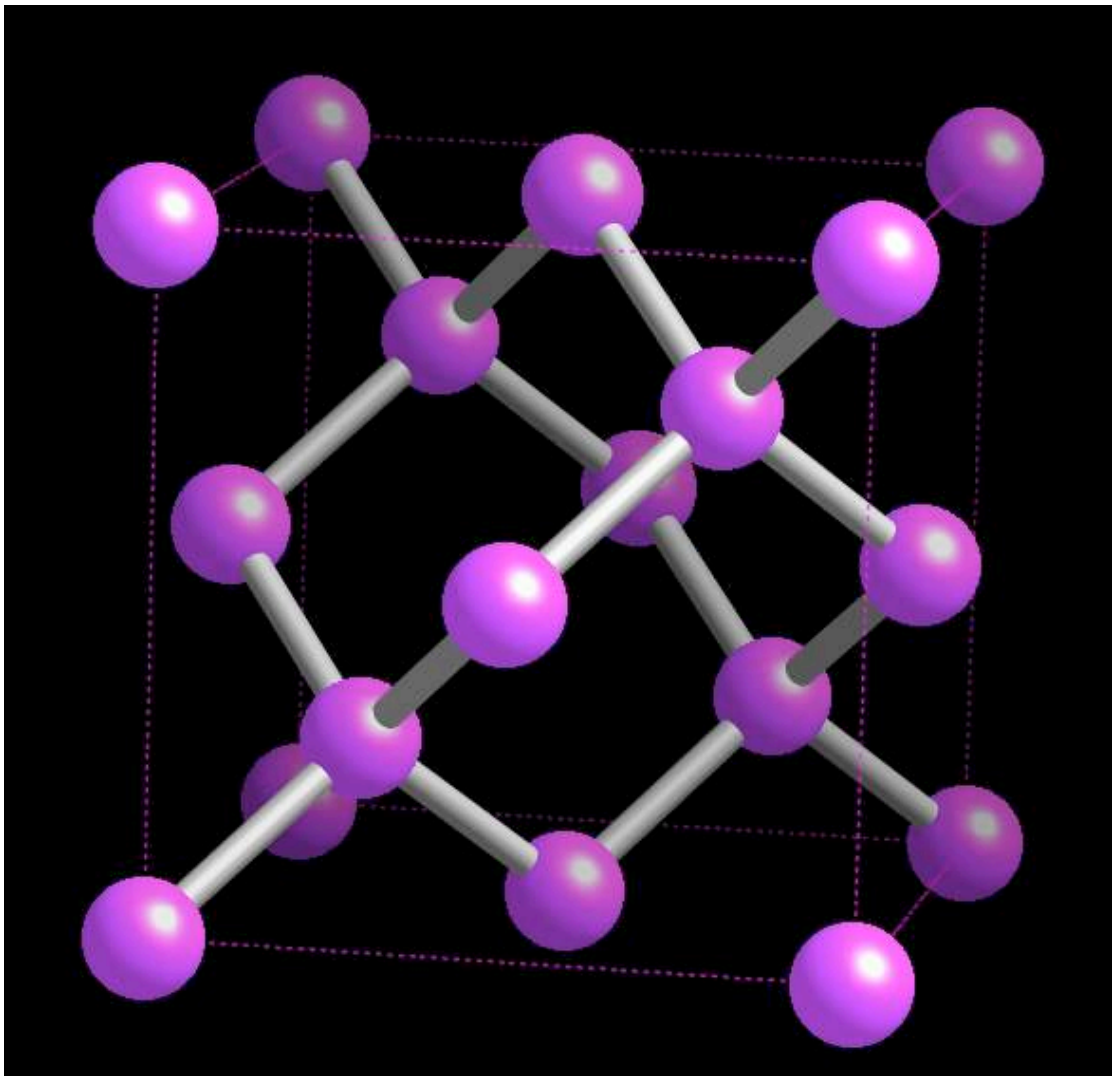
Blue Triangle:

Blue Angle = 180 - 2 x GA

H-C-H angle: 109.47°

Tetrahedral Geometry

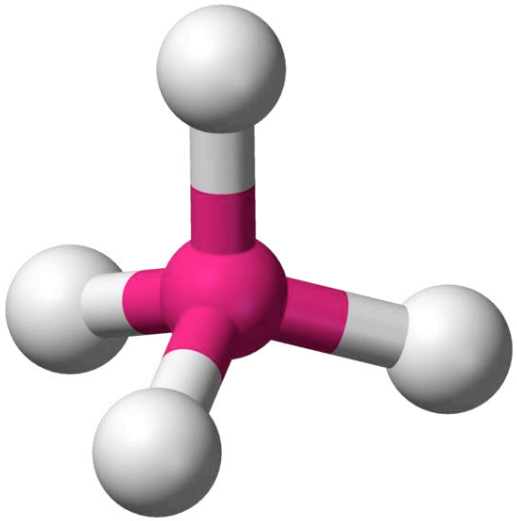
VSEPR in Solids: Diamond Structure



From CrystalMaker

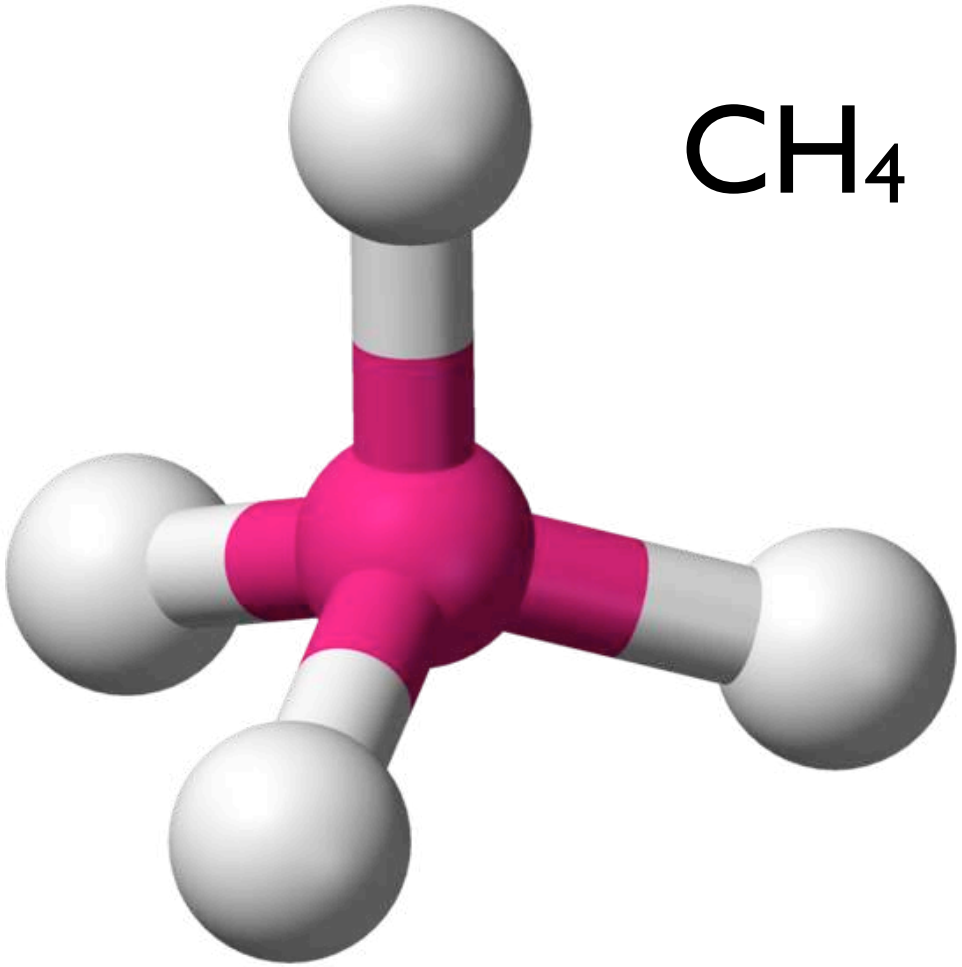
Diamond

Also ZnS



C-C-C angle: 109.47°

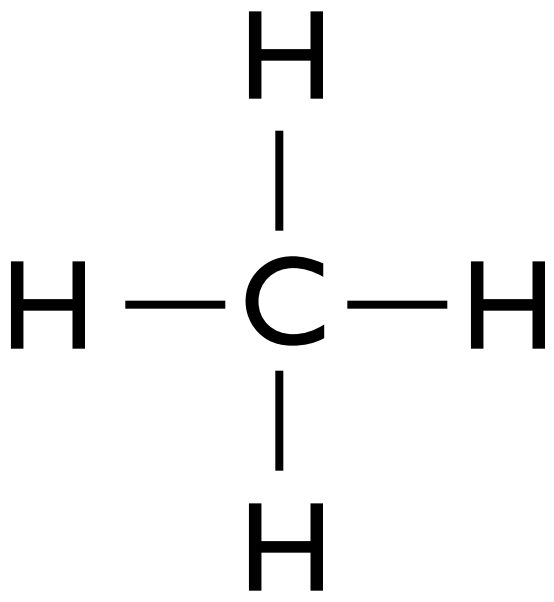
Tetrahedral Site Symmetry



CH_4

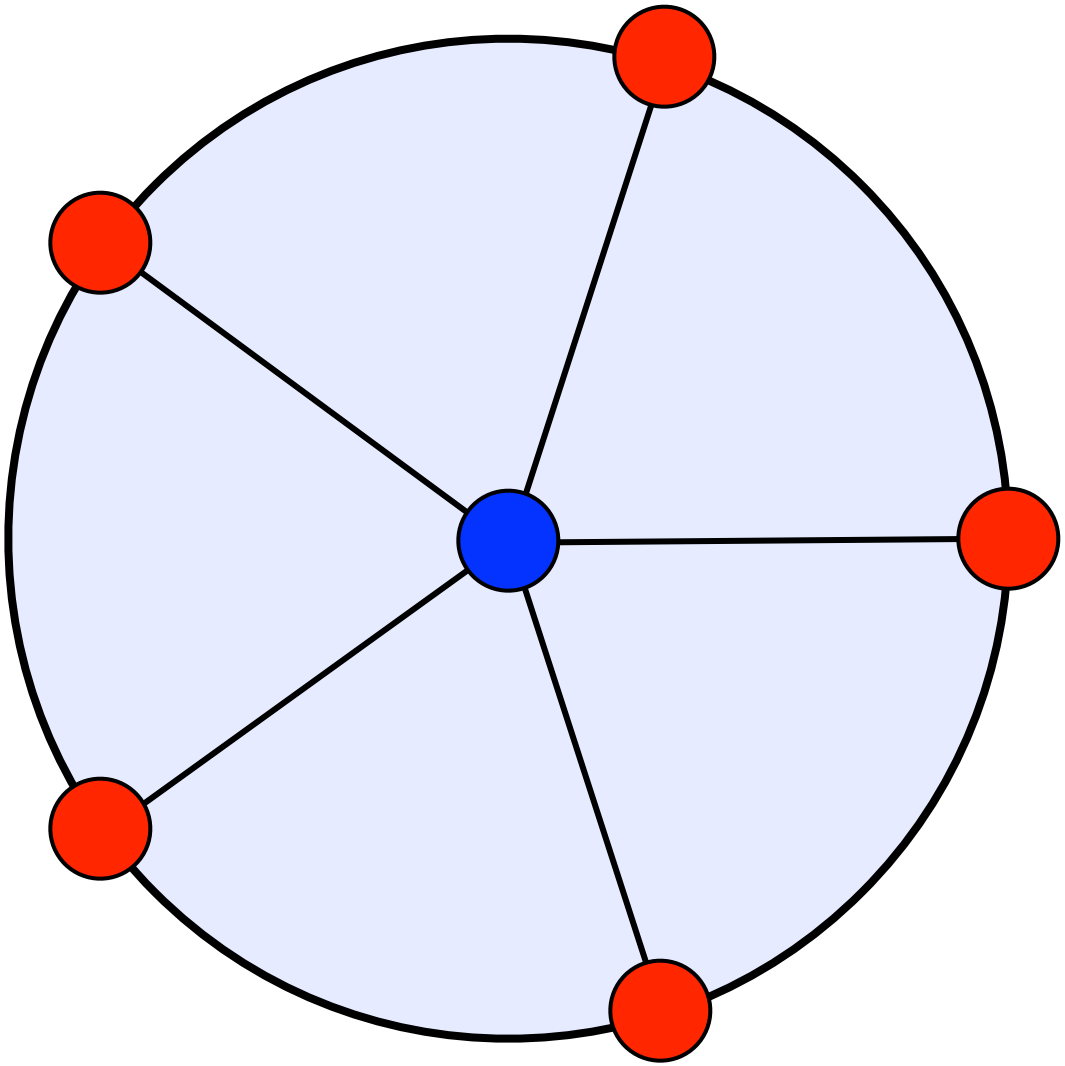
AX_4

8 electrons



H-C-H angle: 109.47°

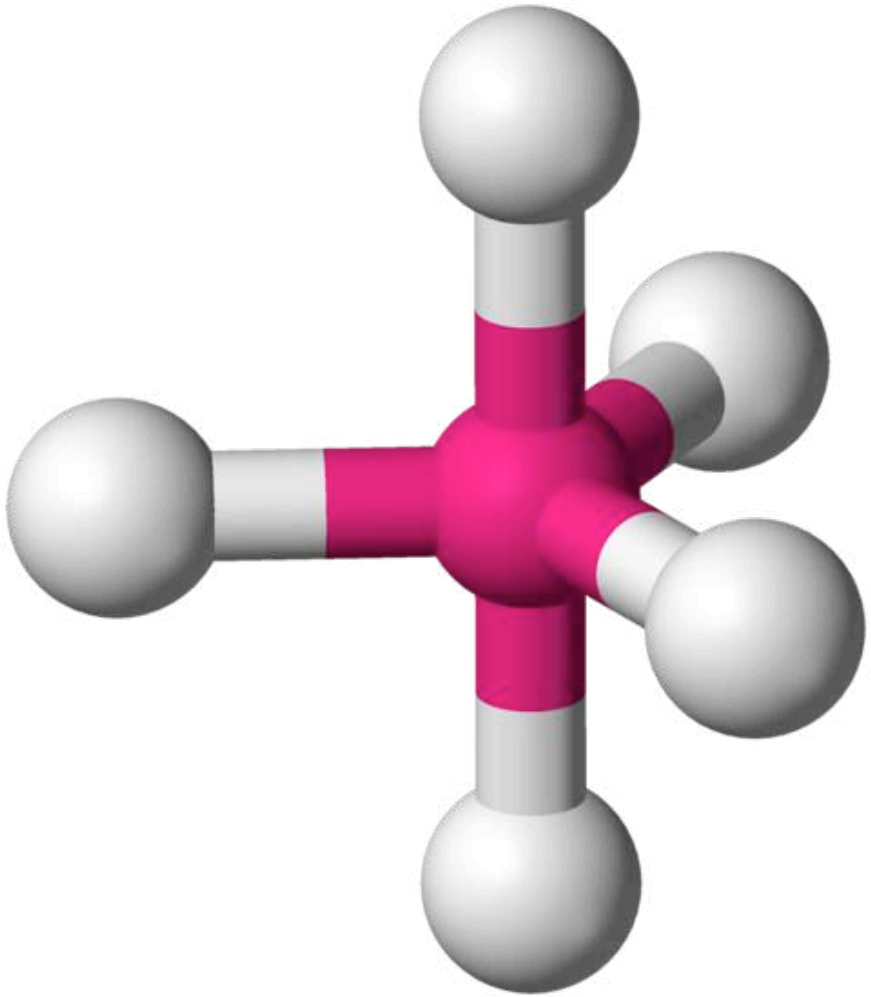
Tetrahedral Geometry



AX_5

X-A-X angle: 72°

Pentagonal Planar Geometry?



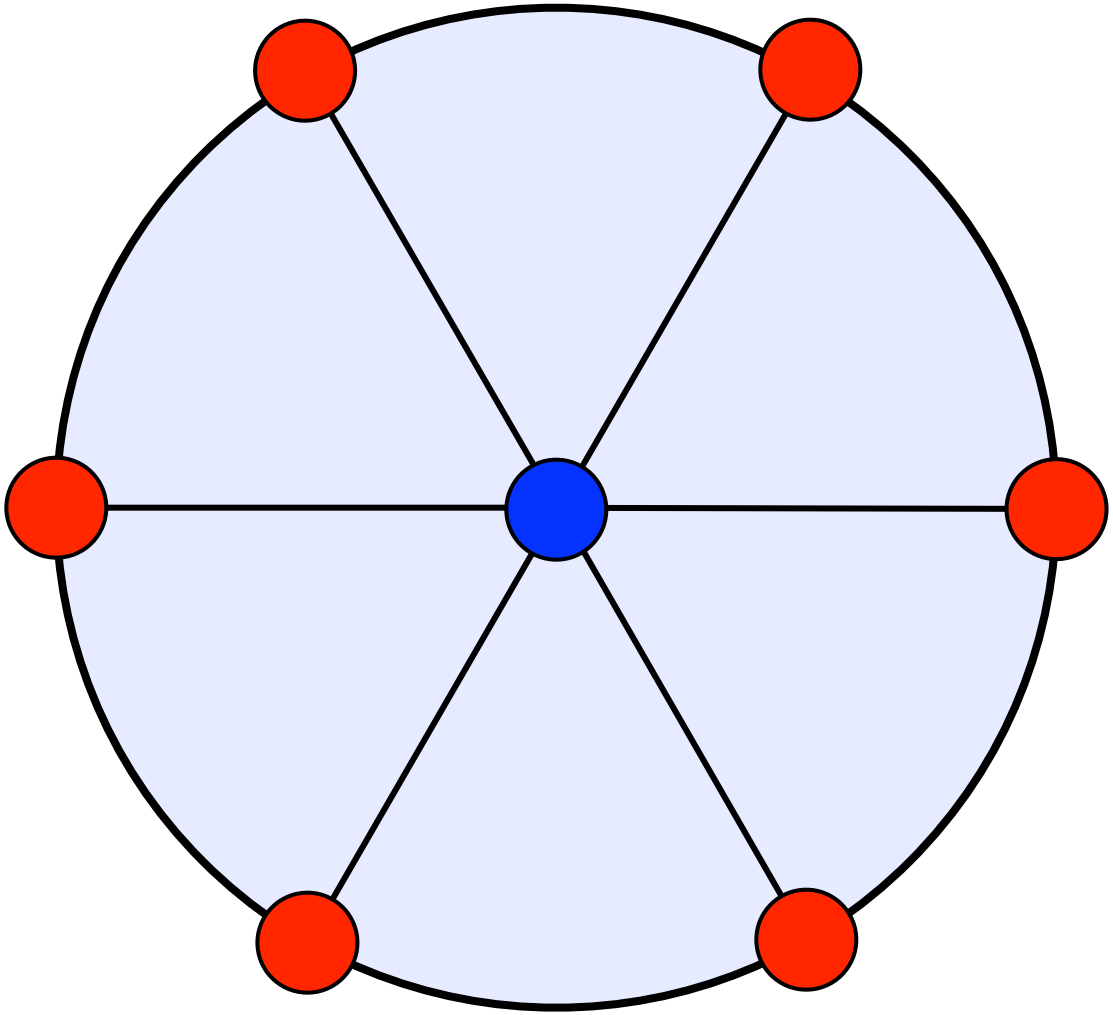
AX_5

PCl_5

40 electrons

Cl-P-Cl angles: 90, 120°

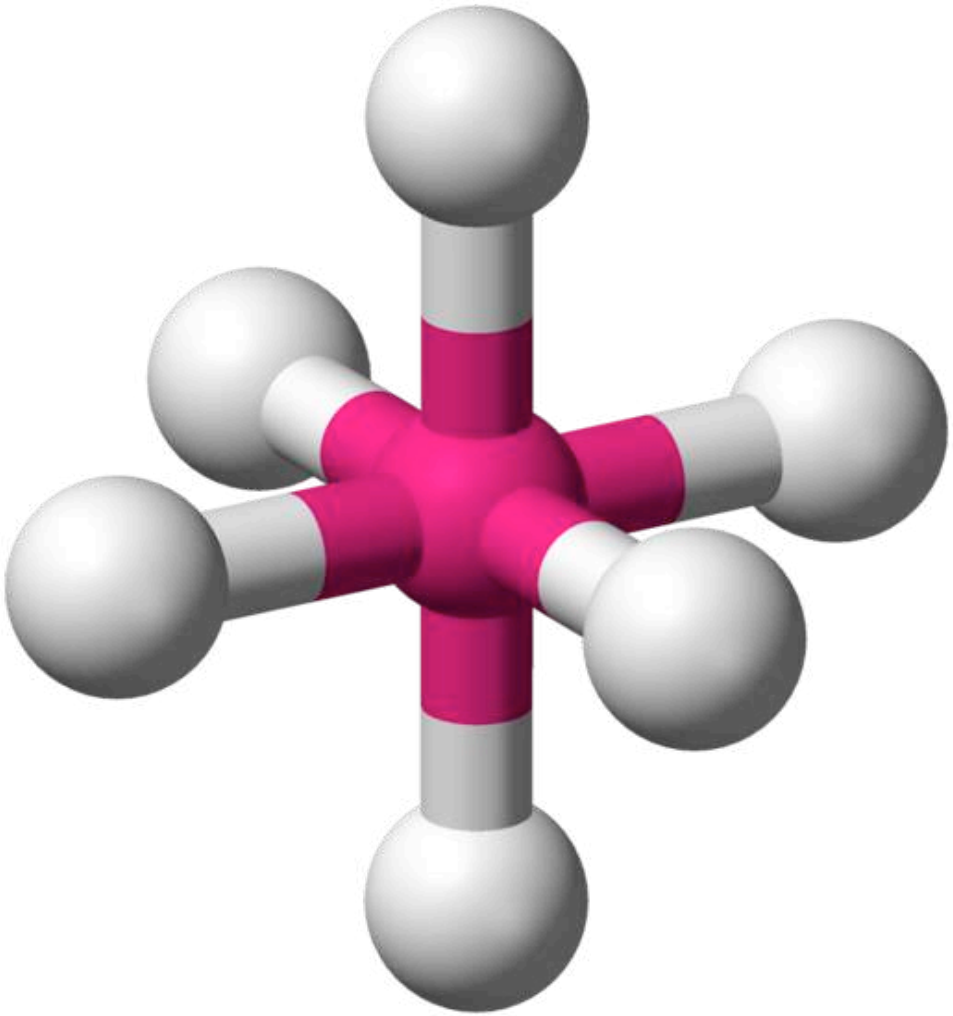
Trigonal Bipyramidal Geometry



AX_6

X-A-X angle: 60°

Hexagonal Geometry?



AX_6

SF_6

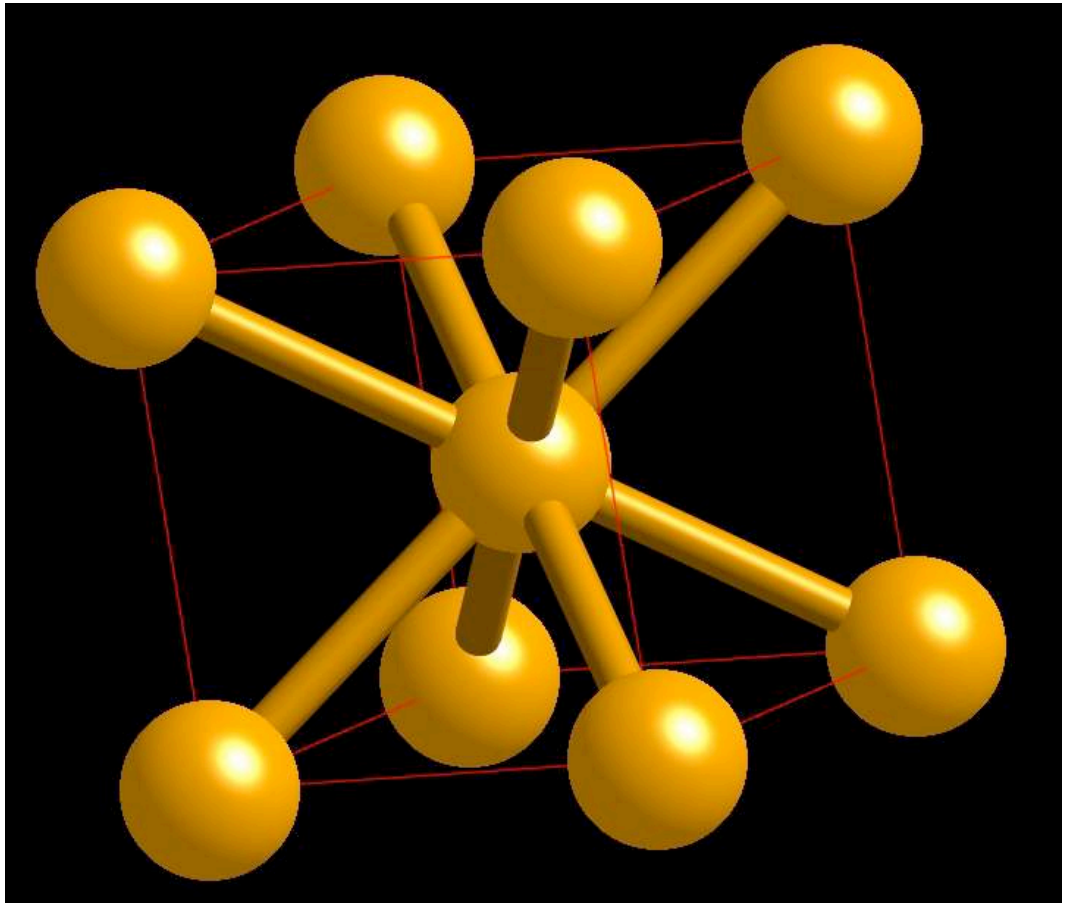
48 electrons

F-S-F angle: 90°

Octahedral Geometry

VSEPR in Solids: Body Centered Cubic Structure

AX_6



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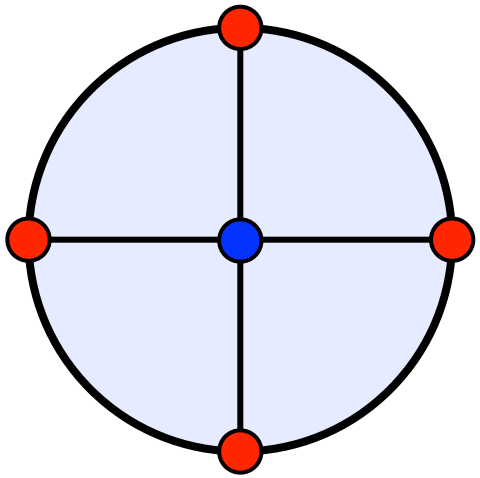

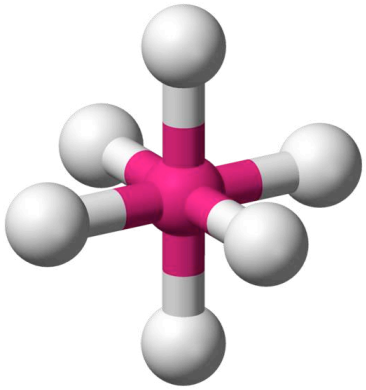

C-C-C angle: 90°

Octahedral Site Symmetry