Molecular Geometry

Molecular Geometry

the three dimensional arrangement of atoms in a molecule

a molecules geometry affects its physical and chemical properties

we can use Lewis structures to predict overall geometries

Repulsions

The most stable arrangement of groups attached to a central atom is the one that has the maximum separation of electron pairs (bonded or nonbonded).

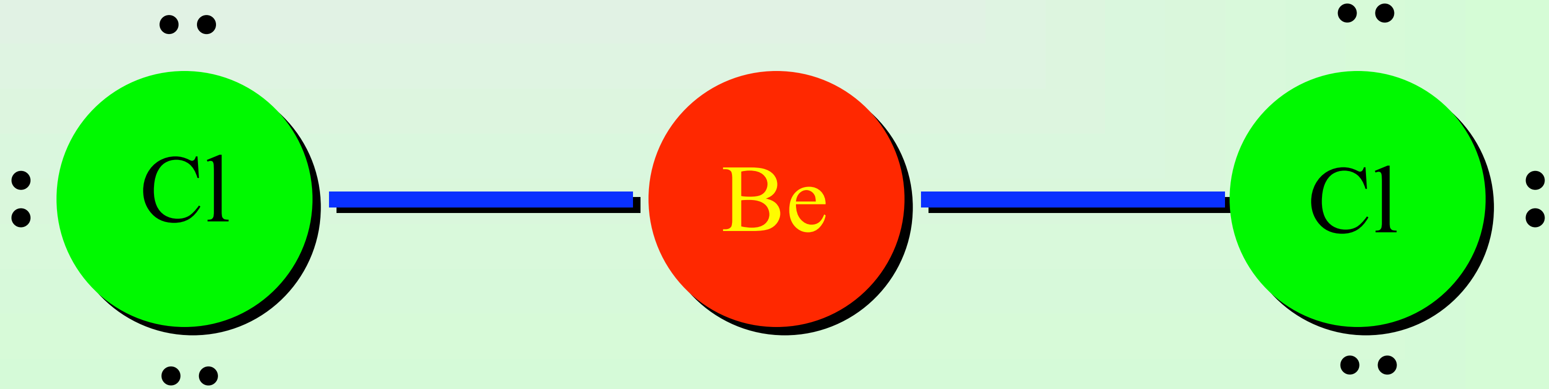
Molecules in Which the Central Atom Has No Lone Pairs

Two Electron Pairs

Beryllium dichloride ($BeCl_2$)

Cl—Be—Cl angle = 180°

linear geometry

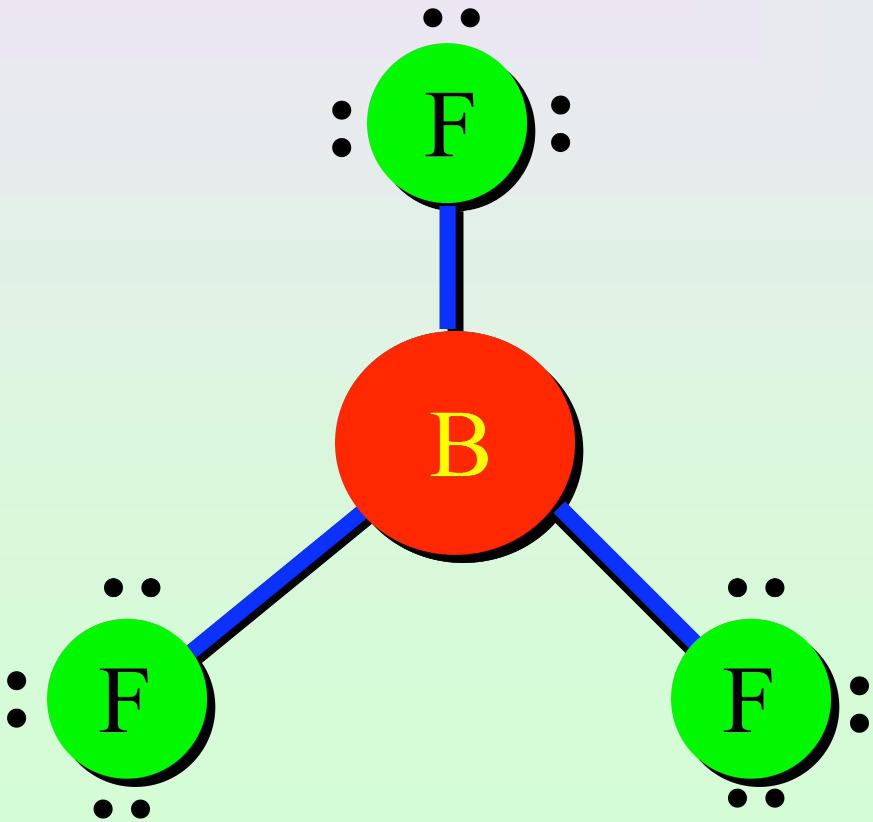


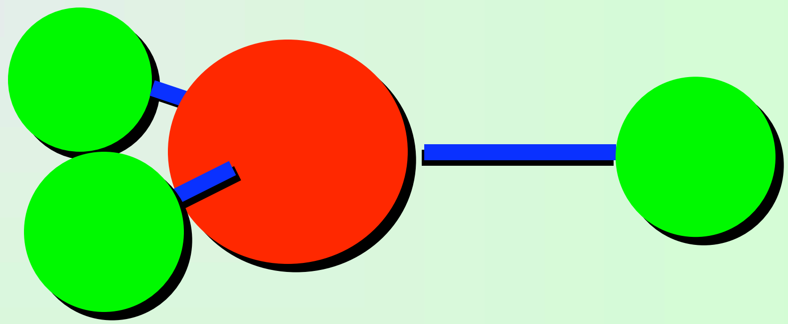
Three Electron Pairs

Boron trifluoride (BF_3)

F—B—F angle = 120 °

trigonal planar geometry



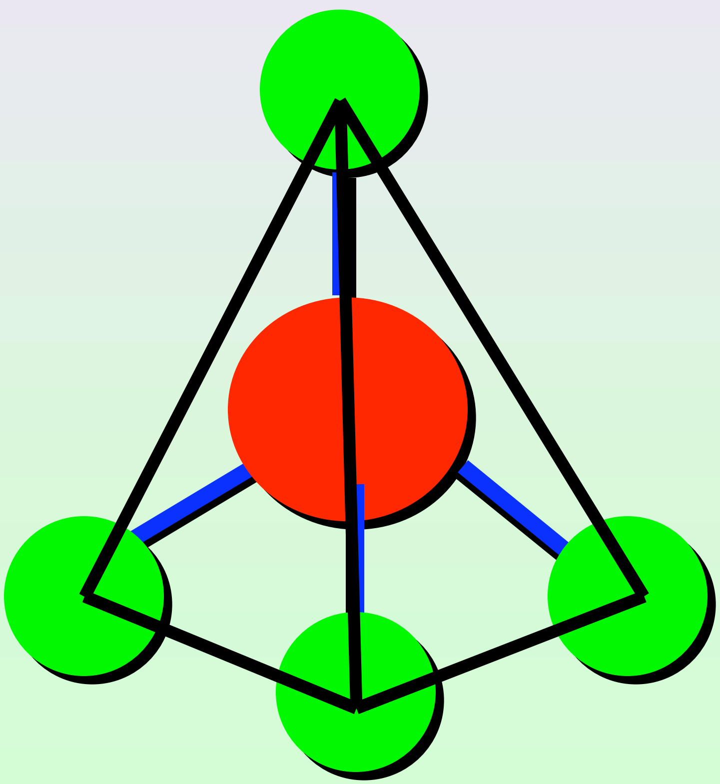


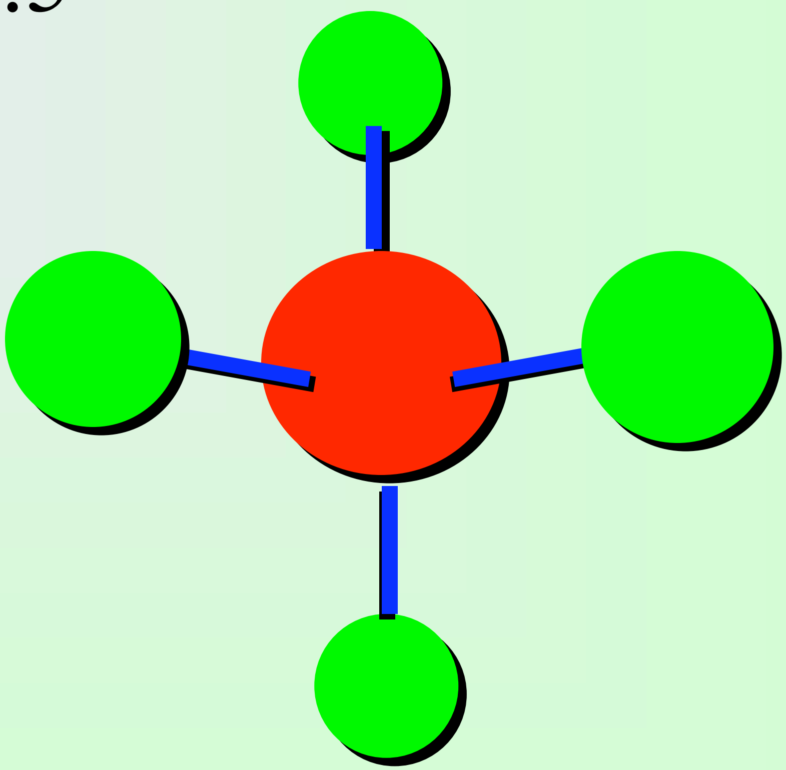
Four Electron Pairs

Methane (CH_4)

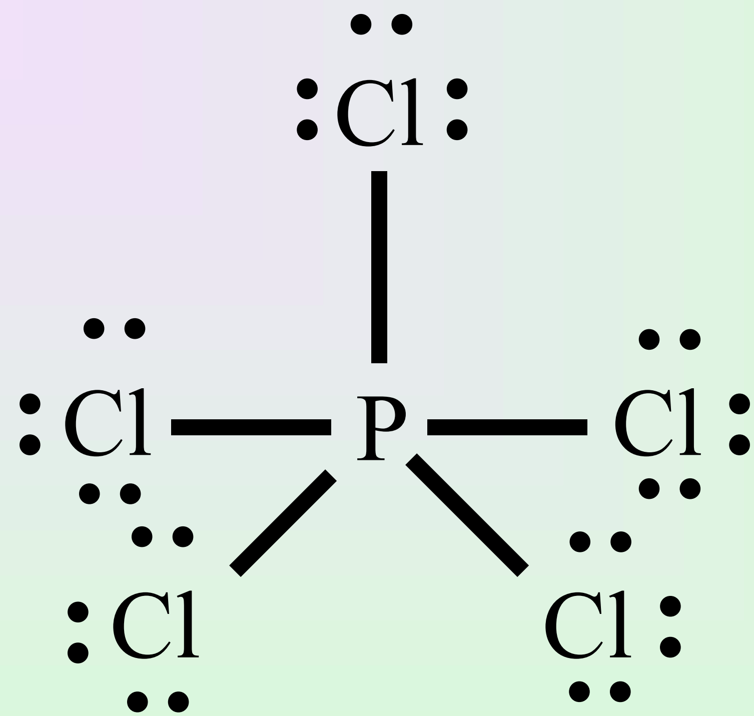
tetrahedral geometry

H—C—H angle = 109.5 °





Phosphorous pentachloride (PCl_5)

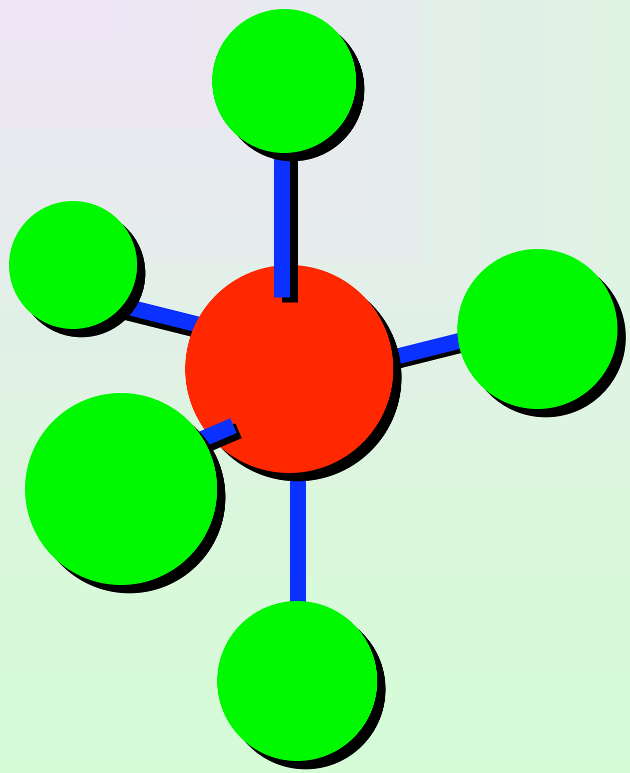


40 electrons

Five electron pairs

Phosphorous pentachloride (PCl_5)

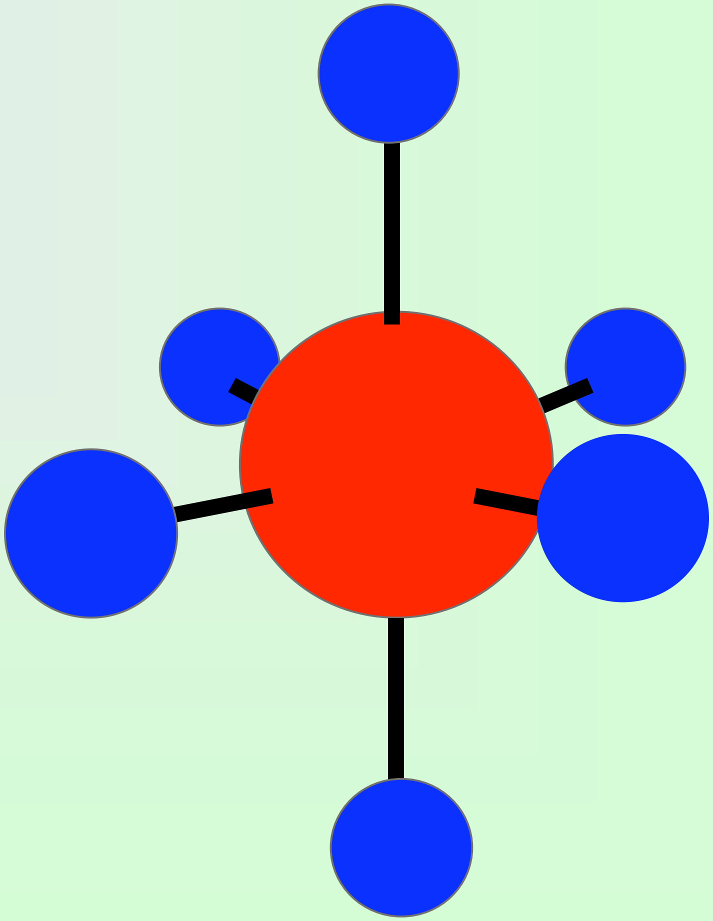
Trigonal bipyramidal geometry



Six electron pairs

Sulfur hexafluoride (SF_6)
octahedral geometry

or
square bipyramidal
geometry

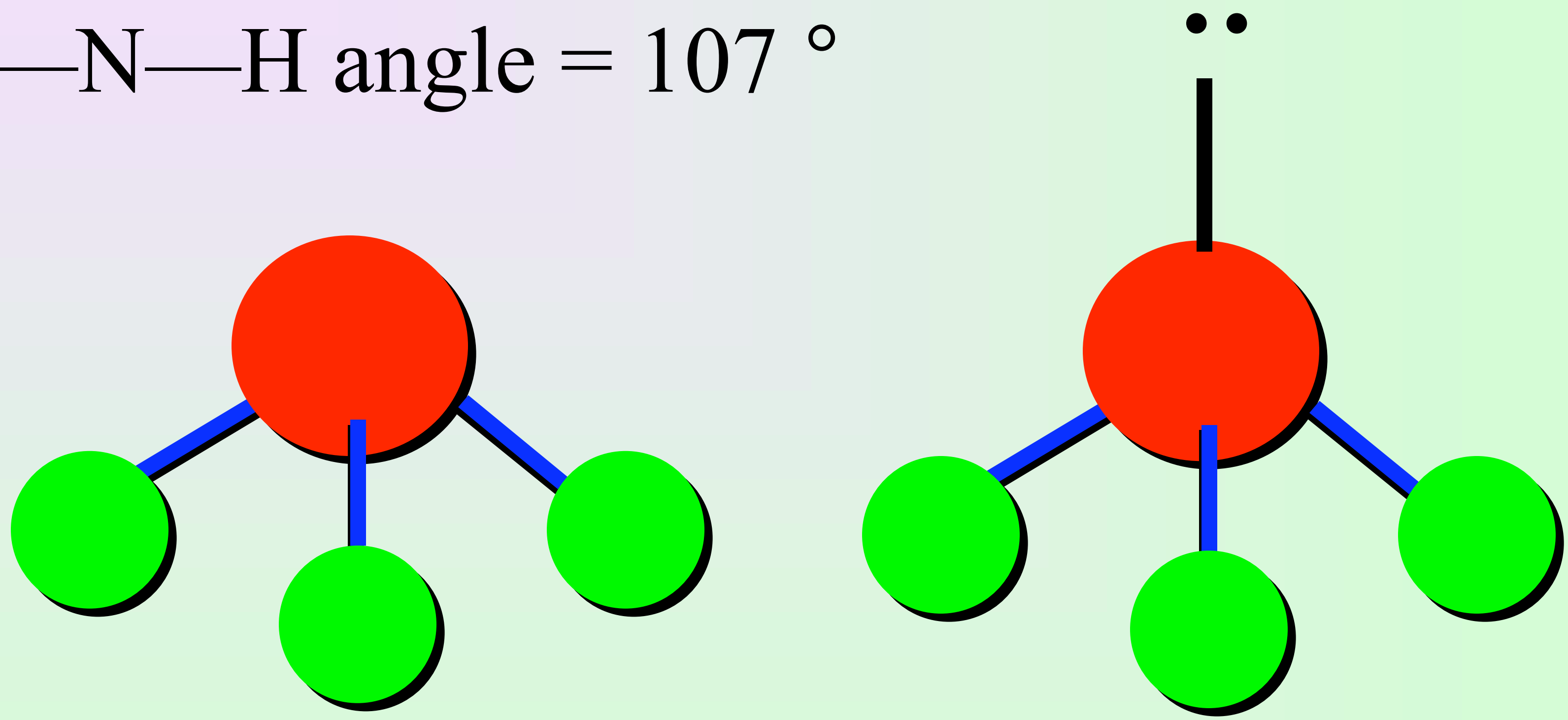


Molecules in which the Central Atom Has One or More Lone Pairs

Ammonia NH_3

trigonal pyramidal geometry

H—N—H angle = 107 °

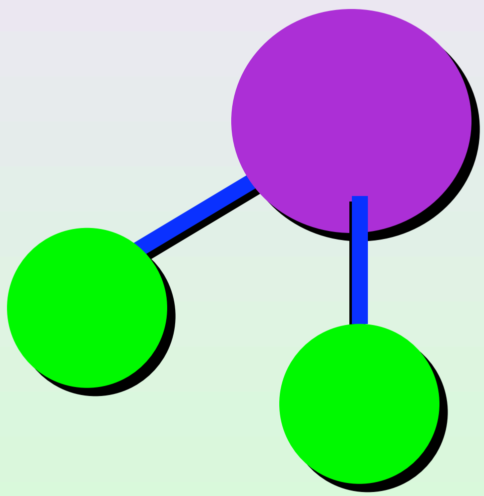


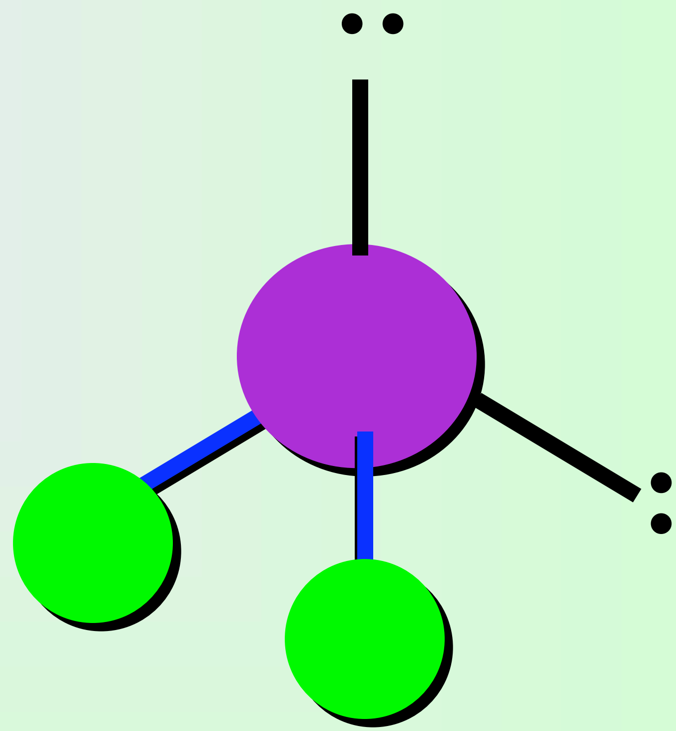
but notice the tetrahedral arrangement of electron pairs

Water H_2O

bent geometry

H—O—H angle = 105 °

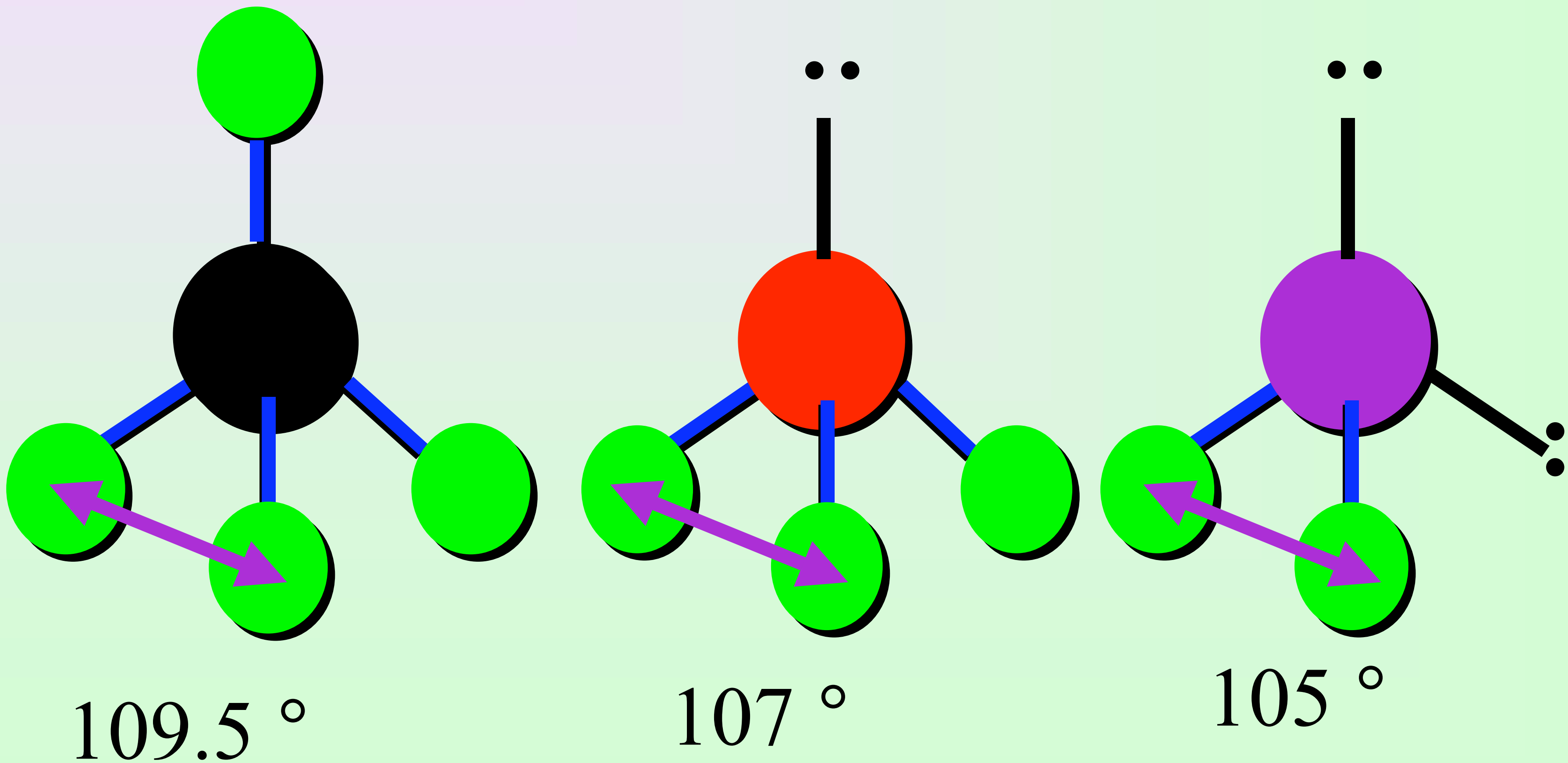




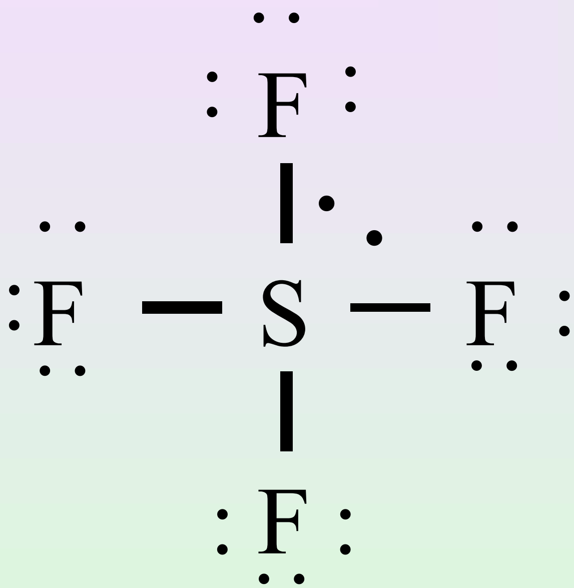
but notice the tetrahedral arrangement of electron pairs

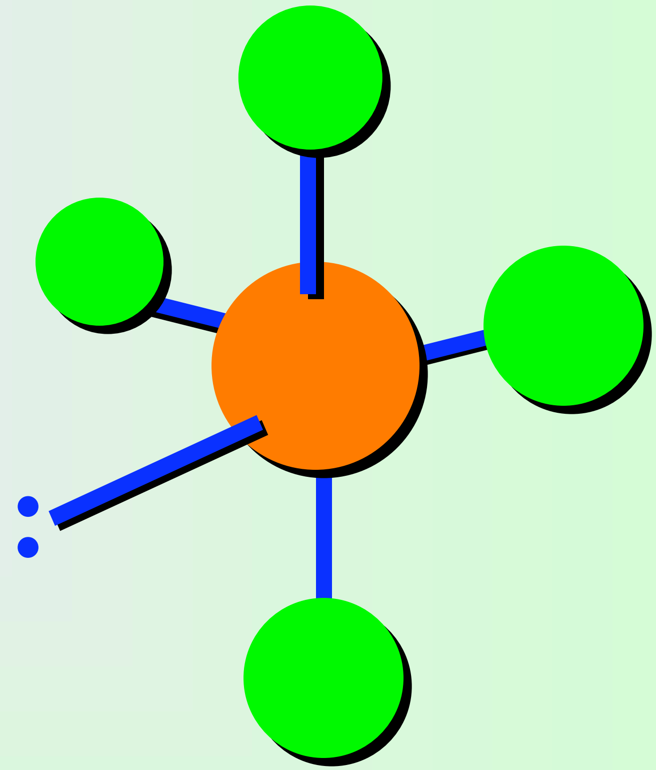
Bond angles in methane, ammonia and water

lone pairs are more repulsive than bonded pairs



Sulfur tetrafluoride (SF_4)

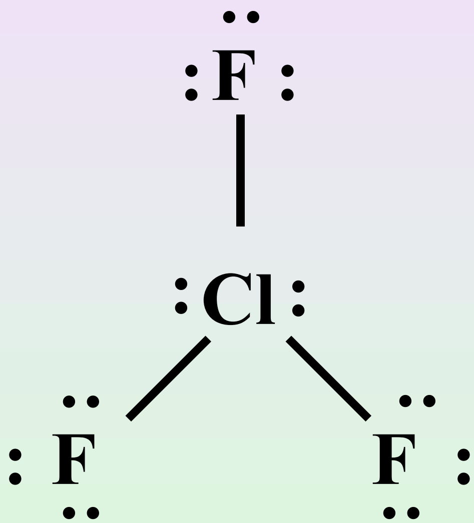




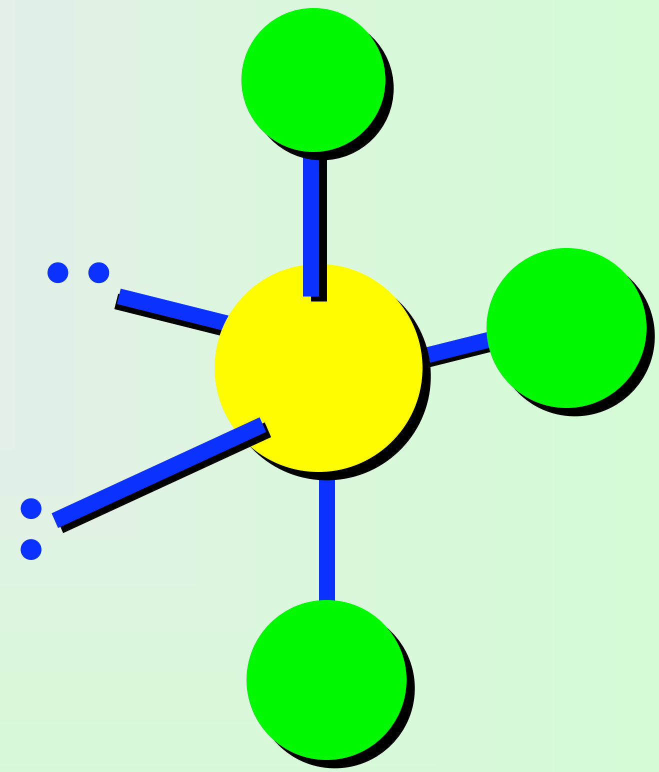
34 electrons
5 electron pairs

seesaw shaped; trigonal bipyramidal arrangement of electron pairs

Chlorine trifluoride



28 electrons
5 electron pairs

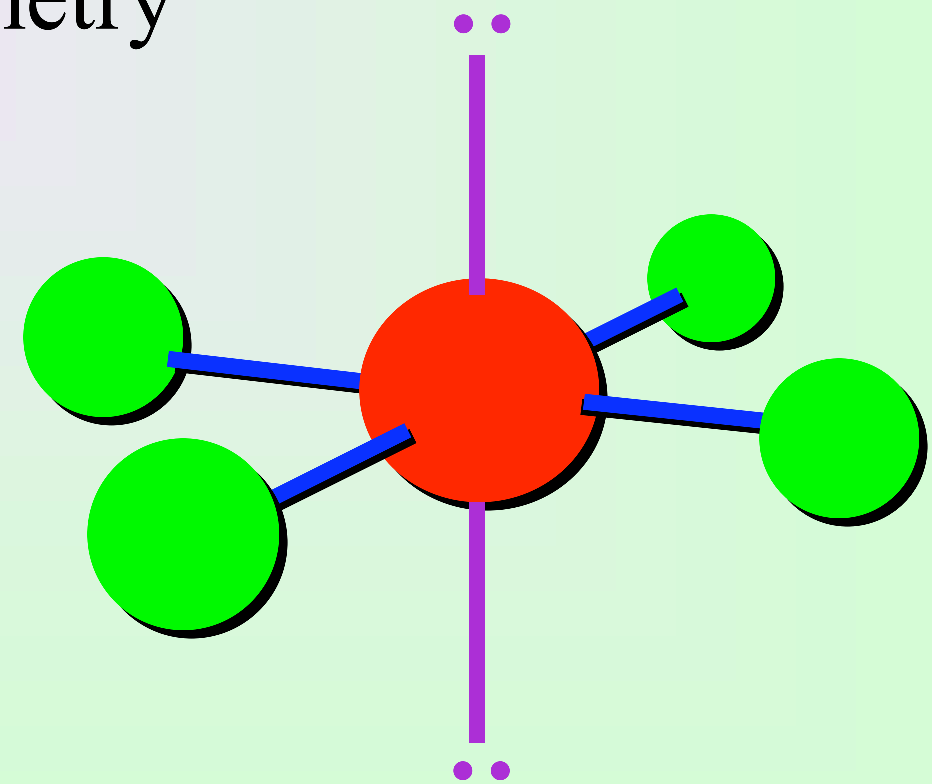


T–shaped

Xenon tetrafluoride

six electrons; octahedral arrangement of electron pairs

square planar geometry

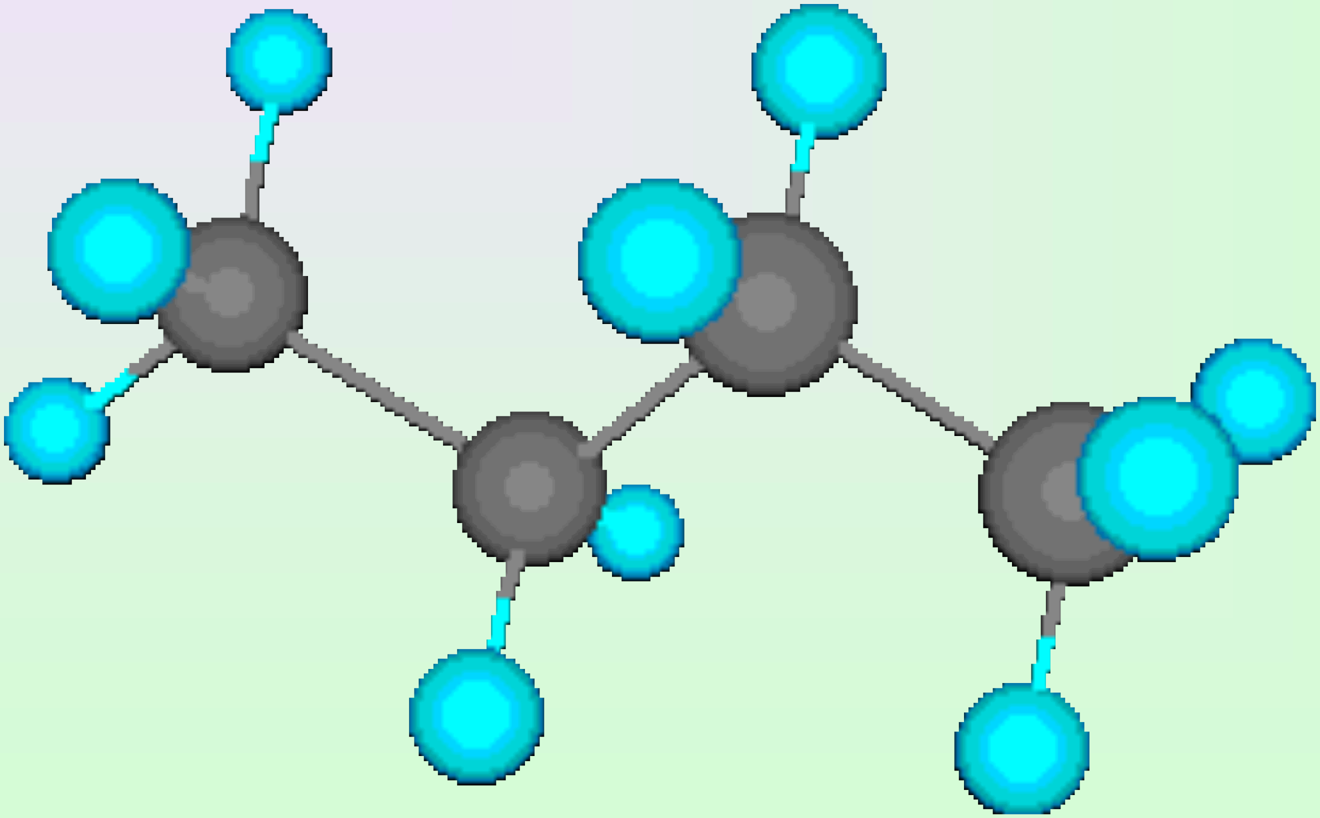


Geometry of Molecules with More Than One Central Atom

Most molecules

lack a “central” atom

therefore, look for local stereochemistry



Guidelines for Applying the VSEPR Model

(Valence-shell electron-pair repulsion)

1) Write the Lewis structure of the molecule.

2) Count the number of electron pairs
around the central atom.

3) Predict geometry of molecule on basis of
maximum separation of electron pairs.

4) Decreasing order of repulsive interactions
    - lone pair-lone pair (most repulsive)
    - lone pair-bonded pair
    - bonded pair-bonded pair (least repulsive)

5) double bonds and triple bonds are treated like
single bonds