

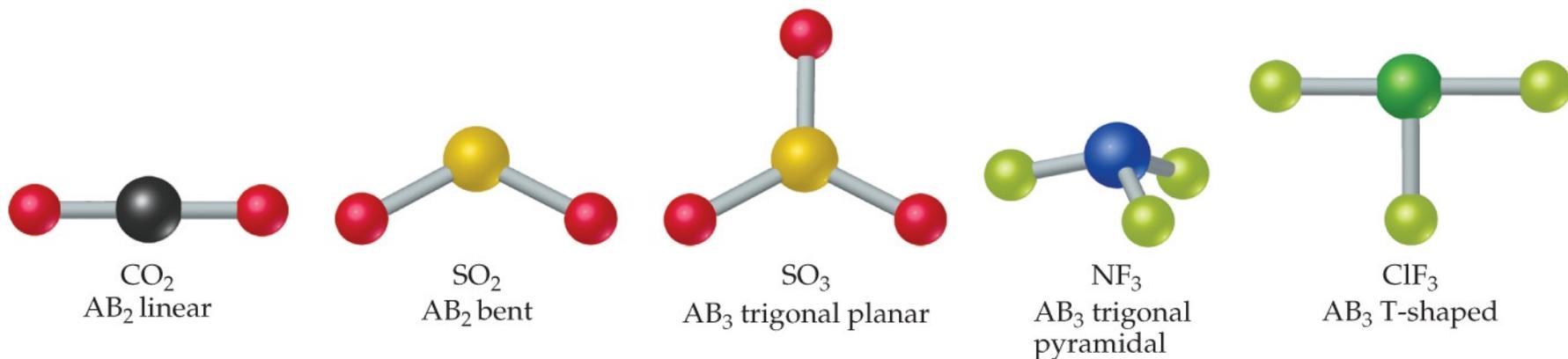
Molecular Geometry

Molecular Geometry

the three dimensional arrangement of atoms in a molecule

a molecule's geometry affects its physical and chemical properties

we can use Lewis structures to predict overall geometries

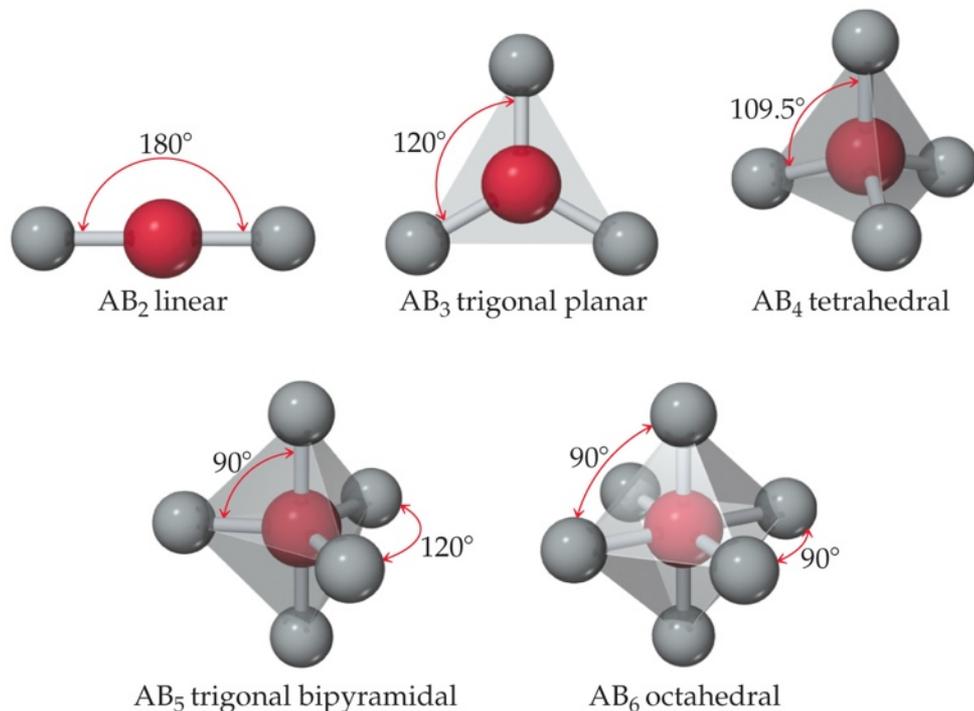


Repulsions

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

What Determines the Shape of a Molecule?

- Simply put, electron pairs, whether they be bonding or nonbonding, repel each other.
- By assuming the electron pairs are placed as far as possible from each other, we can predict the shape of the molecule.



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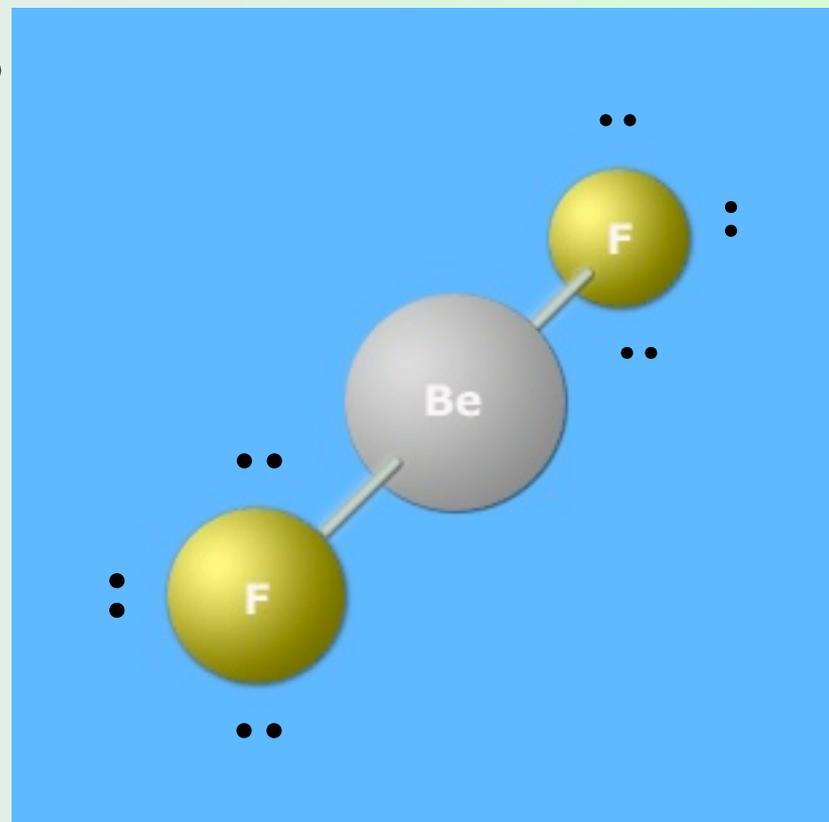
Molecules in Which the Central Atom Has No Lone Pairs

Two Electron Pairs

Beryllium dichloride (BeF_2)

F—Be—F angle = 180°

linear geometry

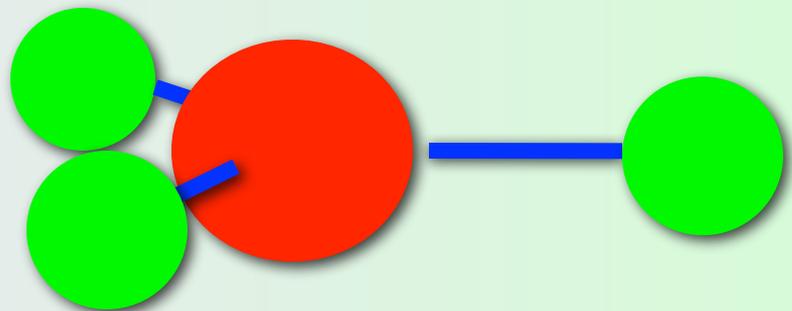
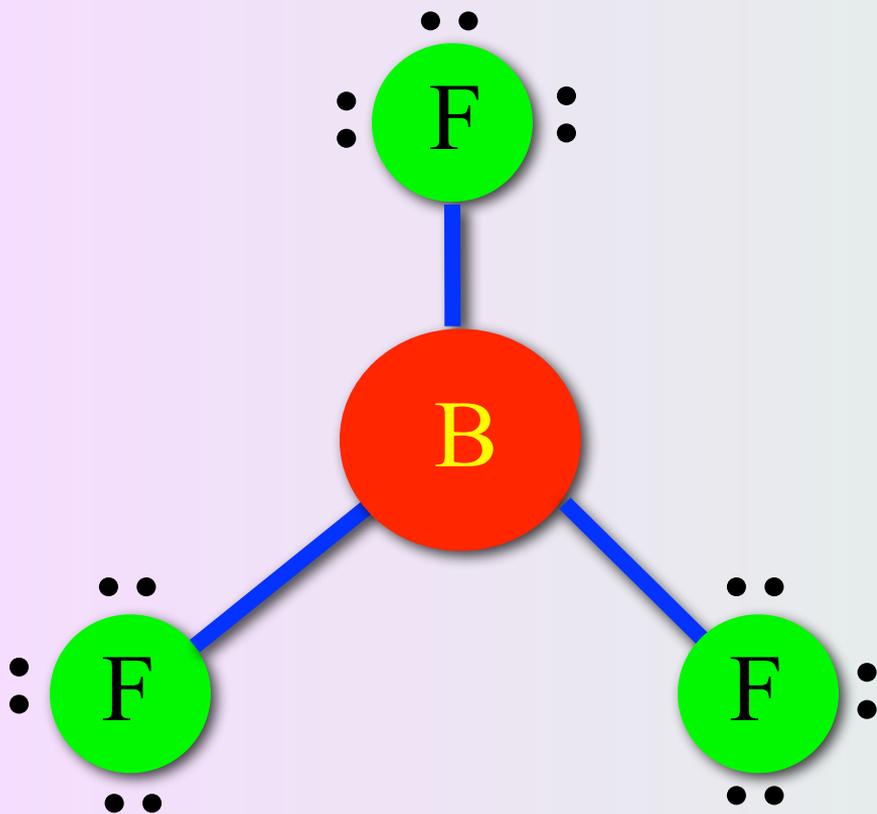


Three Electron Pairs

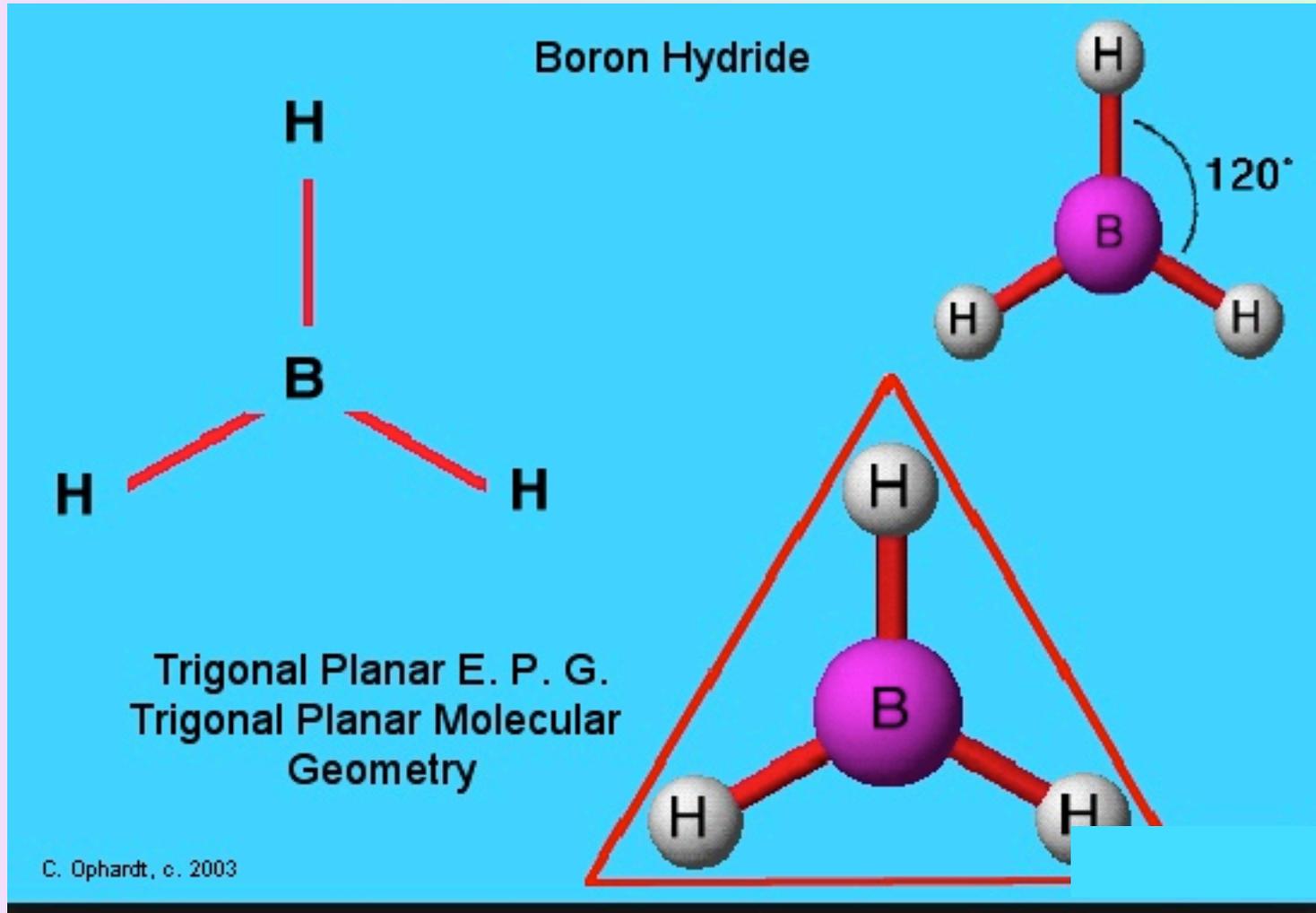
Boron trihydride (BF_3)

F—B—F angle = 120°

trigonal planar geometry



Boron trihydride (BF_3)

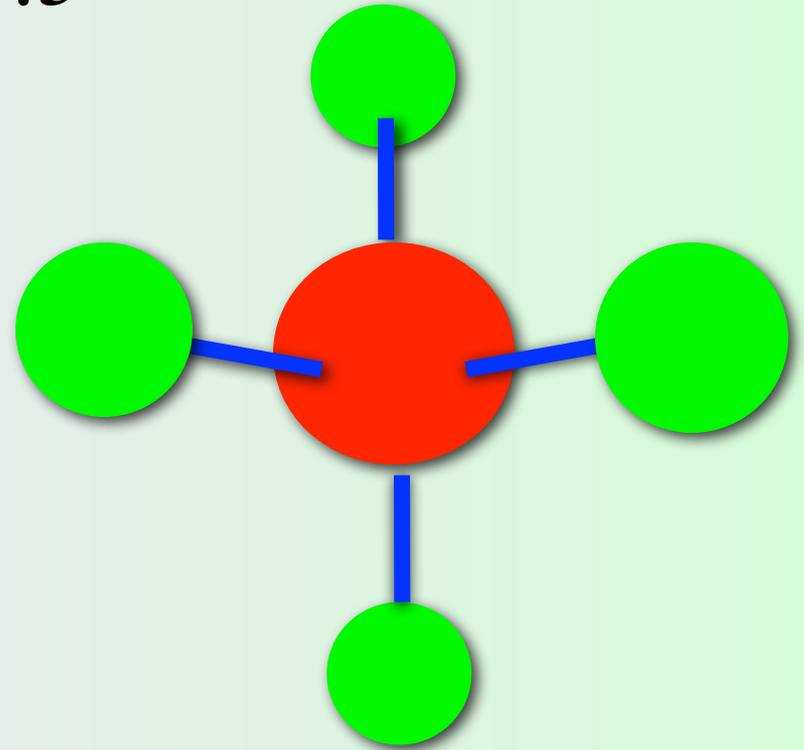
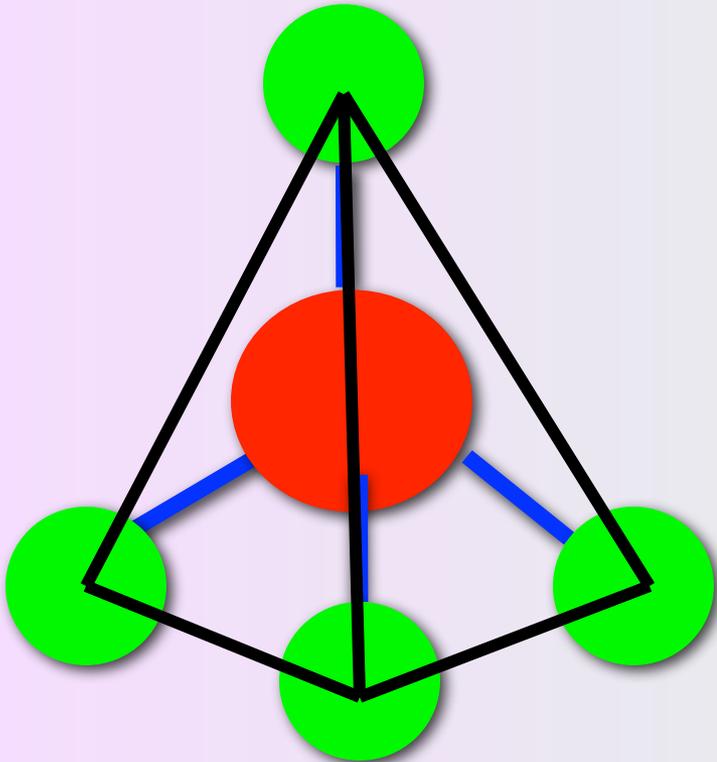


Four Electron Pairs

Methane (CH₄)

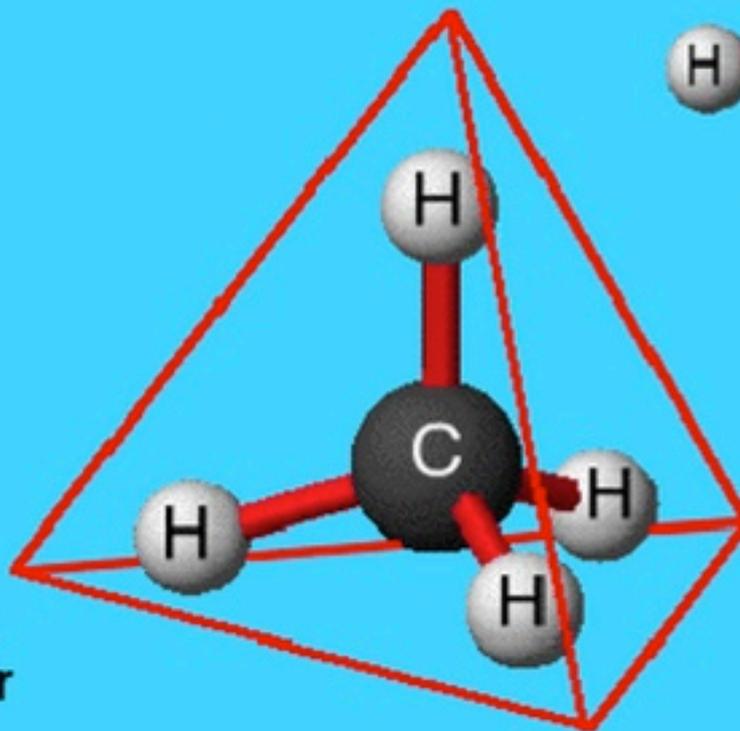
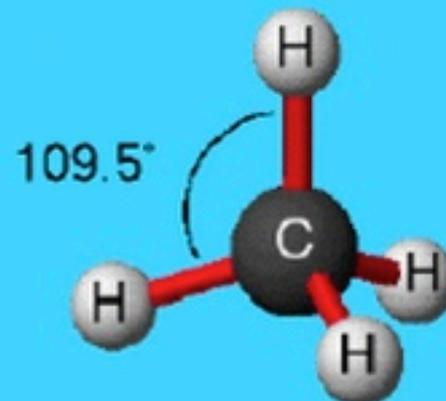
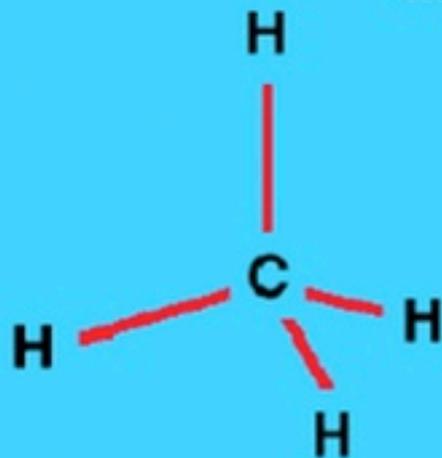
tetrahedral geometry

H—C—H angle = 109.5 °



Methane (CH₄)

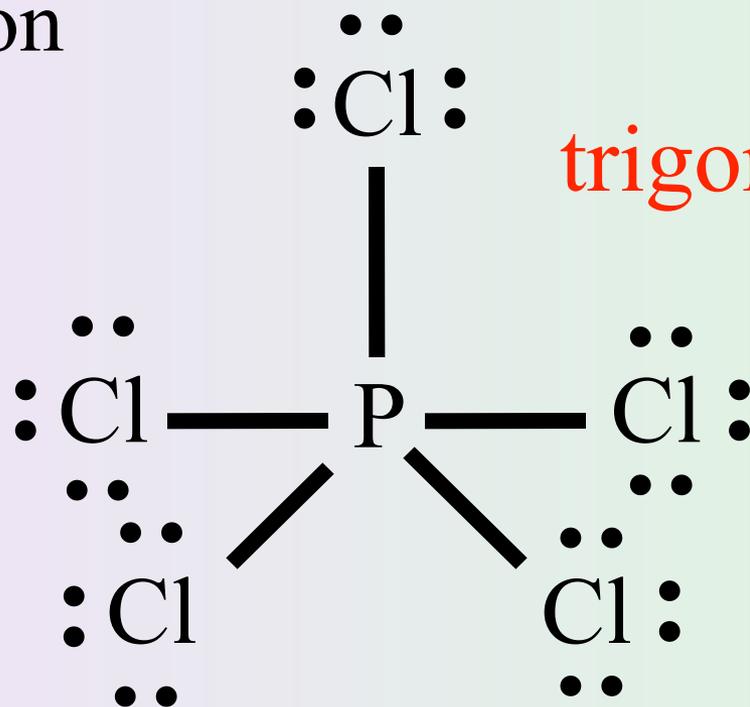
Methane



Tetrahedral E. P. G.
Tetrahedral Molecular
Geometry

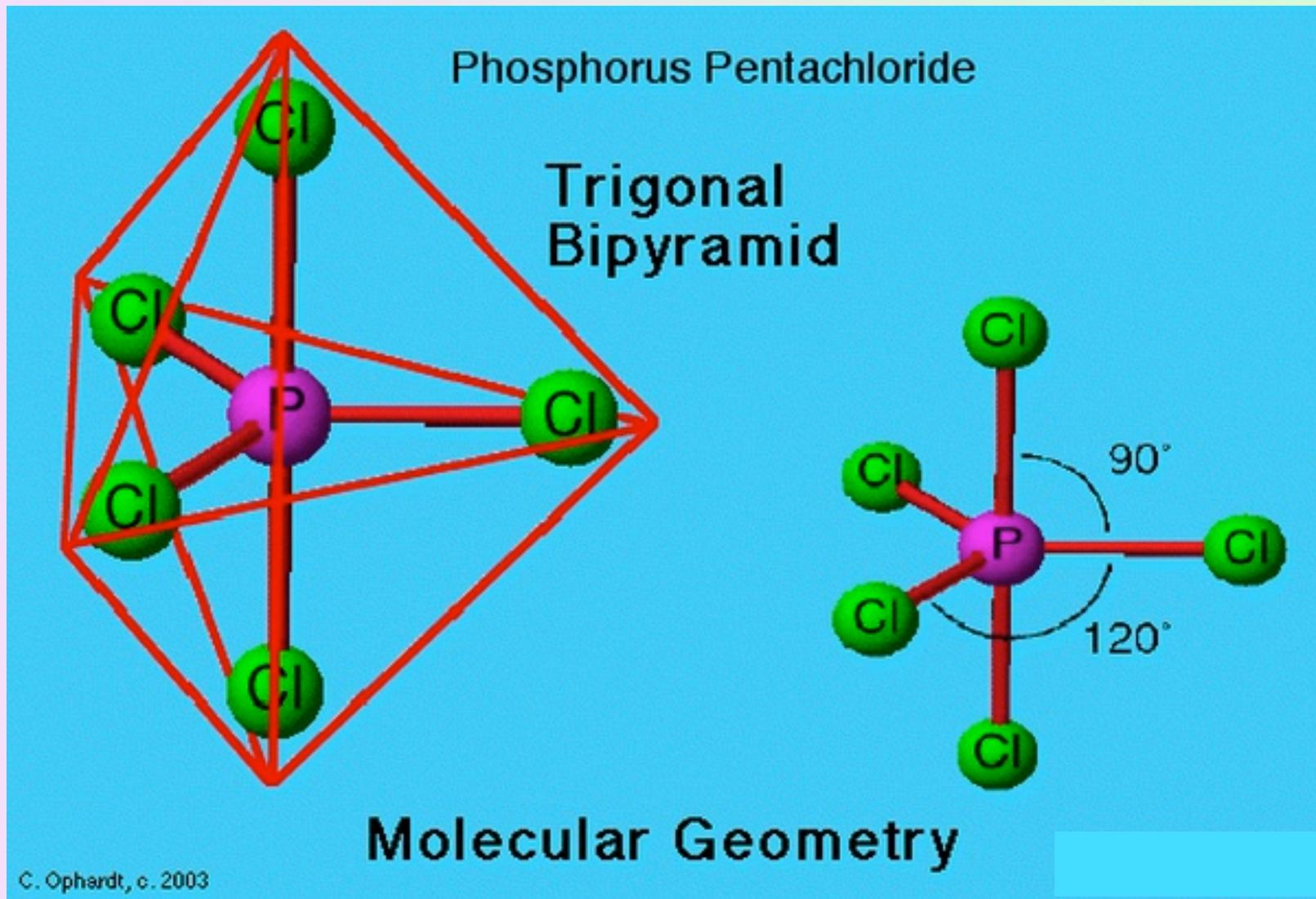
Phosphorous pentachloride (PCl₅)

Five electron
pairs



40 electrons

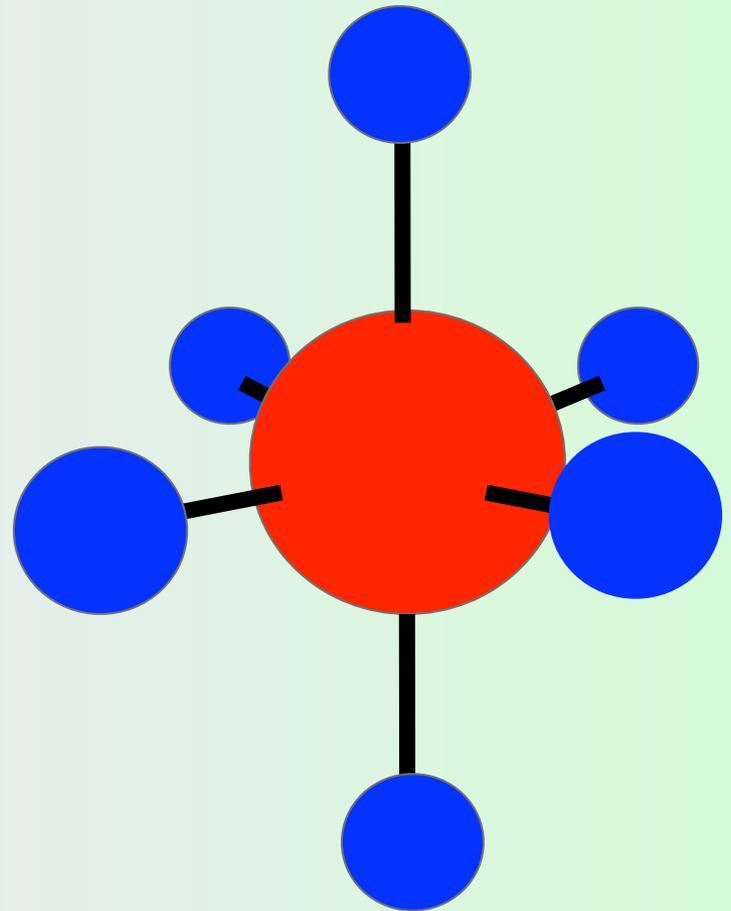
Phosphorous pentachloride (PCl_5)



Six electron pairs

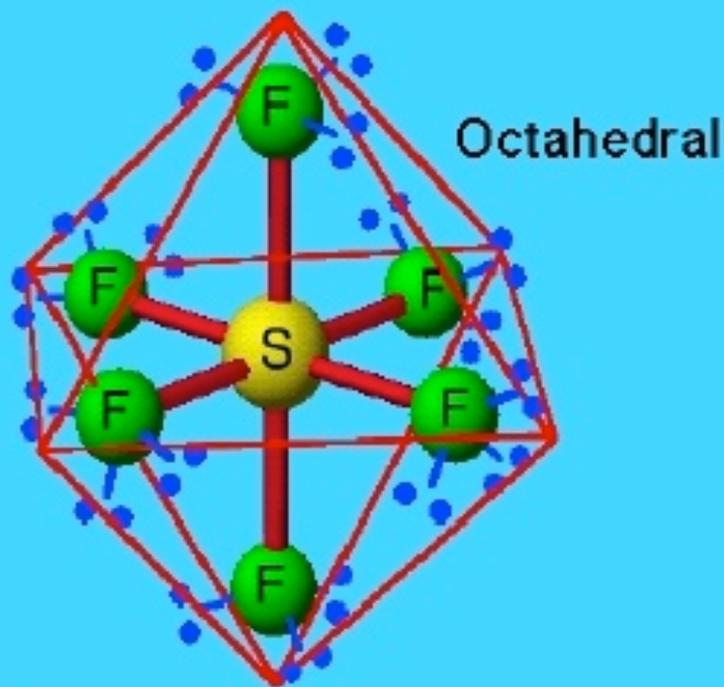
Sulfur hexafluoride (SF_6)
octahedral geometry

or
square bipyramidal
geometry



Sulfur hexafluoride (SF_6)

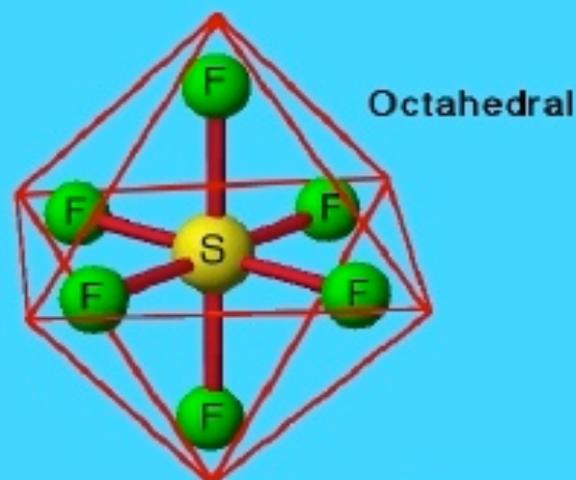
Sulfur Hexafluoride



Electron Pair Geometry



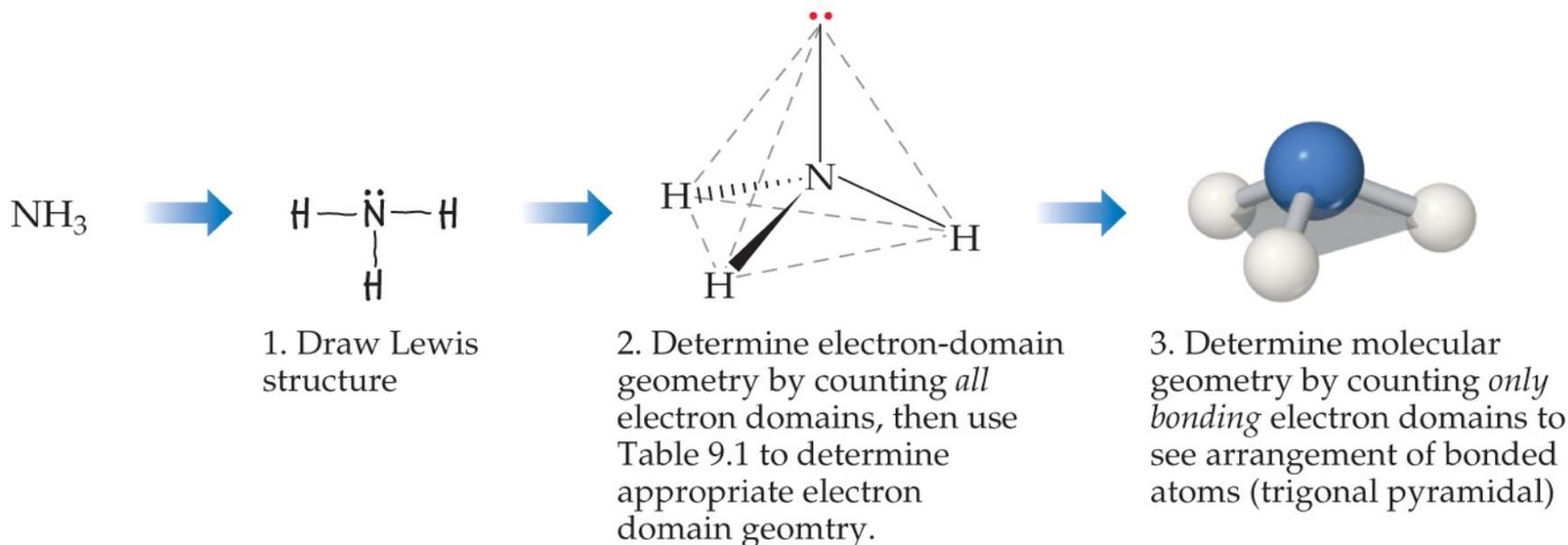
Bond Angles



Molecular Geometry

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

Molecular Geometries



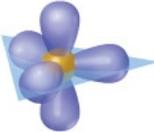
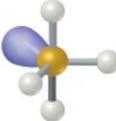
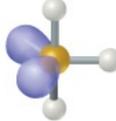
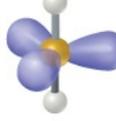
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- The electron-domain geometry is often *not* the shape of the molecule, however.
- The molecular geometry is that defined by the positions of *only* the atoms in the molecules, not the nonbonding pairs.

Trigonal Bipyramidal Electron Domain

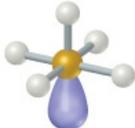
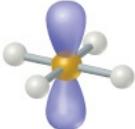
- There are four distinct molecular geometries in this domain:
 - Trigonal bipyramidal
 - Seesaw
 - T-shaped
 - Linear

TABLE 9.3 • Electron-Domain and Molecular Geometries for Five and Six Electron Domains around a Central Atom

Number of Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
5	 Trigonal bipyramidal	5	0	 Trigonal bipyramidal	PCl ₅
		4	1	 Seesaw	SF ₄
		3	2	 T-shaped	ClF ₃
		2	3	 Linear	XeF ₂

Octahedral Electron Domain

TABLE 9.3 • Electron-Domain and Molecular Geometries for Five and Six Electron Domains around a Central Atom

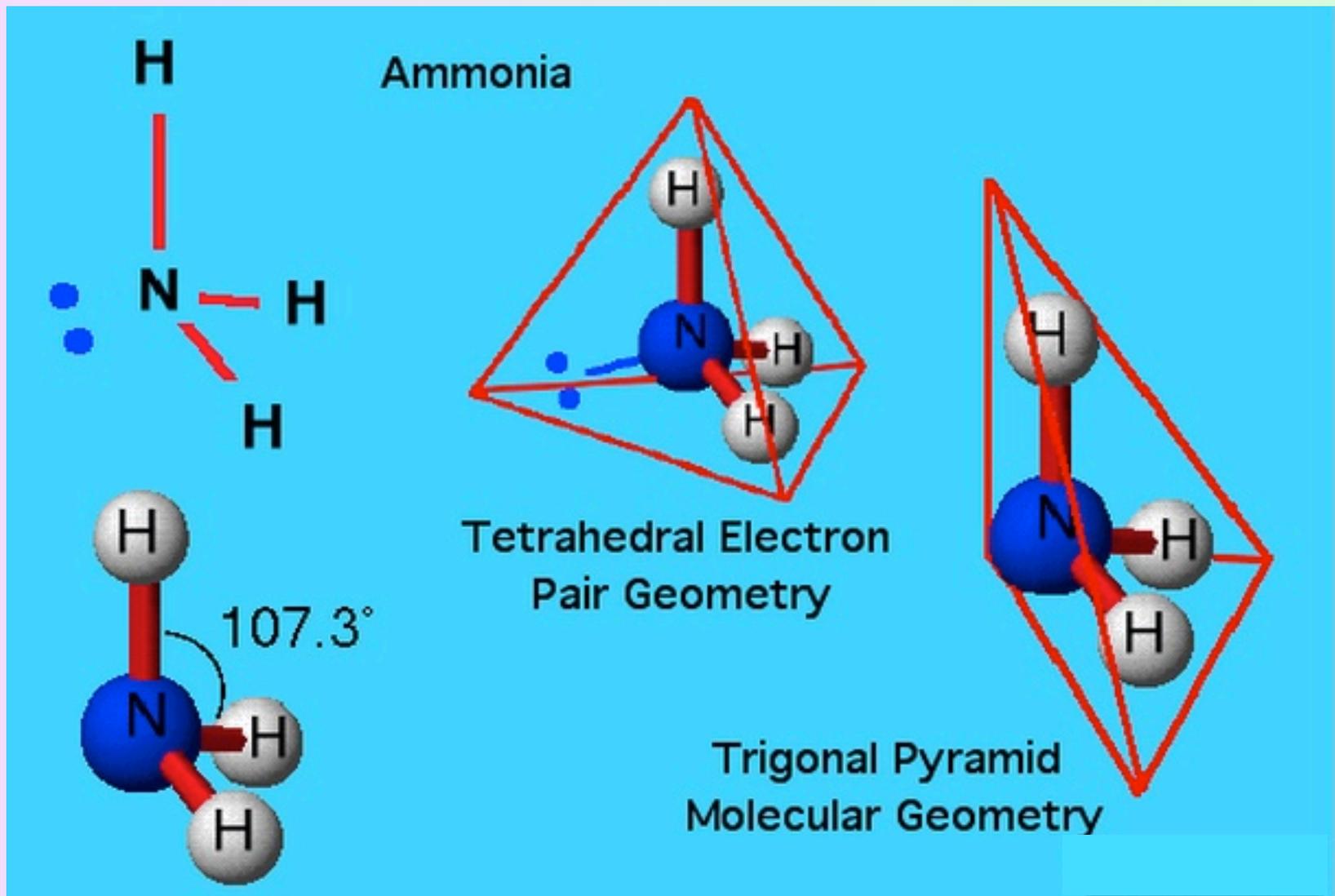
Number of Electron Domains	Electron-Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
6	 Octahedral	6	0	 Octahedral	SF ₆
		5	1	 Square pyramidal	BrF ₅
		4	2	 Square planar	XeF ₄

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- All positions are equivalent in the octahedral domain.
- There are three molecular geometries:
 - Octahedral
 - Square pyramidal
 - Square planar

Ammonia NH_3

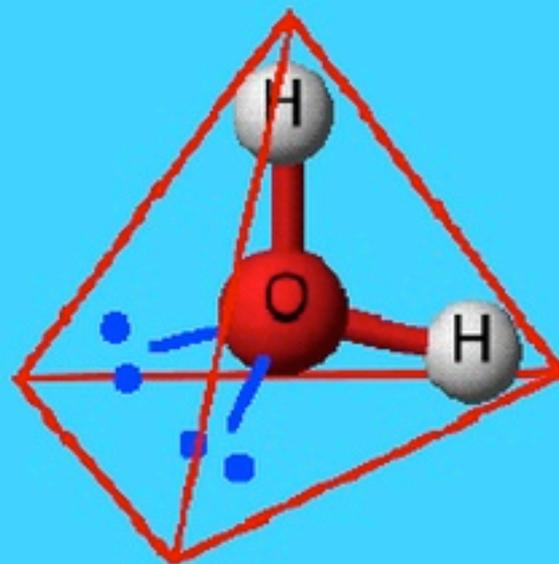
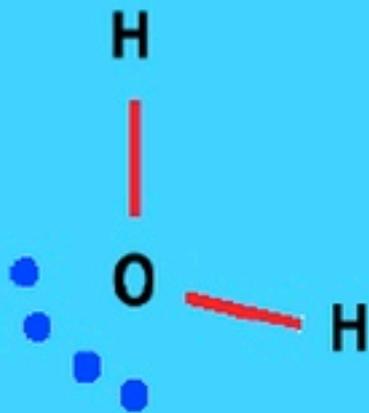
trigonal pyramidal



Water H_2O

bent

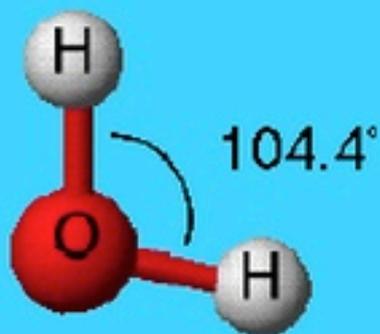
Water



Tetrahedral Electron Pair Geometry

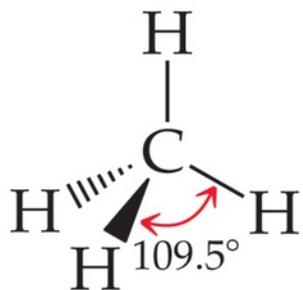


Bent Molecular Geometry

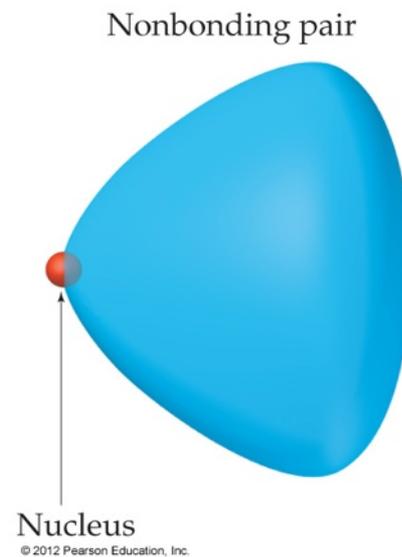
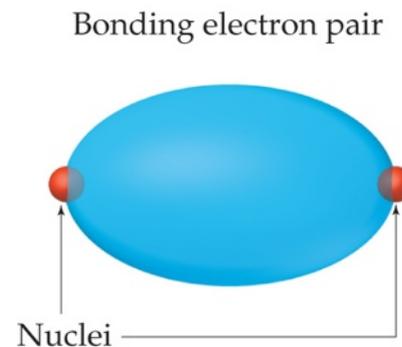
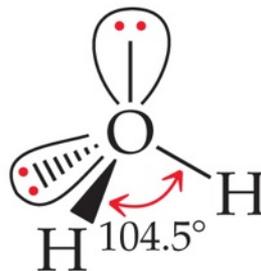
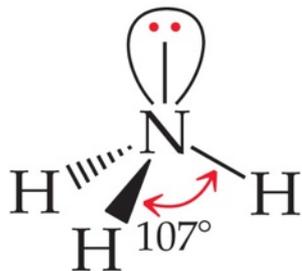


Nonbonding Pairs and Bond Angle

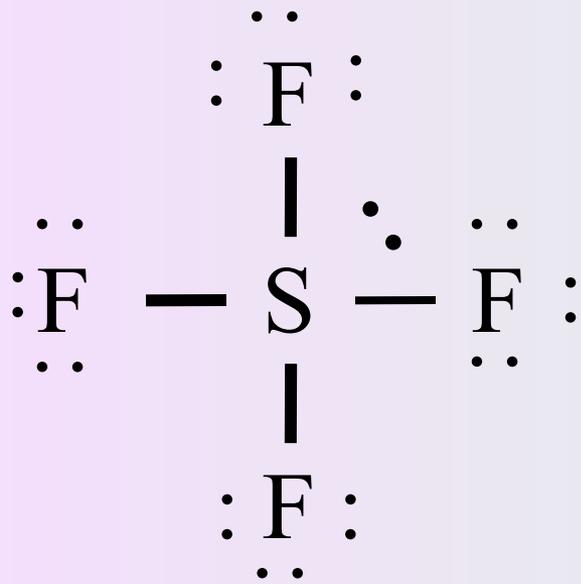
- Nonbonding pairs are physically larger than bonding pairs.
- Therefore, their repulsions are greater; this tends to decrease bond angles in a molecule.



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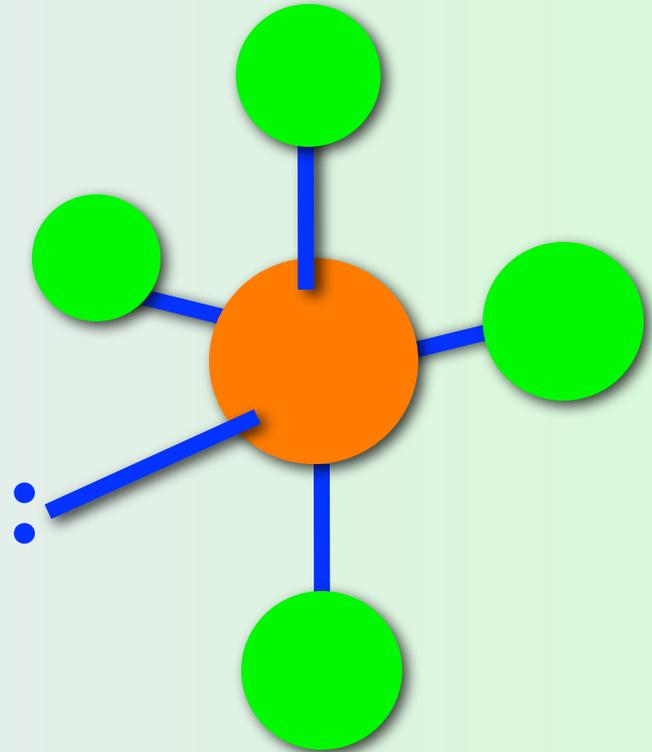


Sulfur tetrafluoride (SF₄)



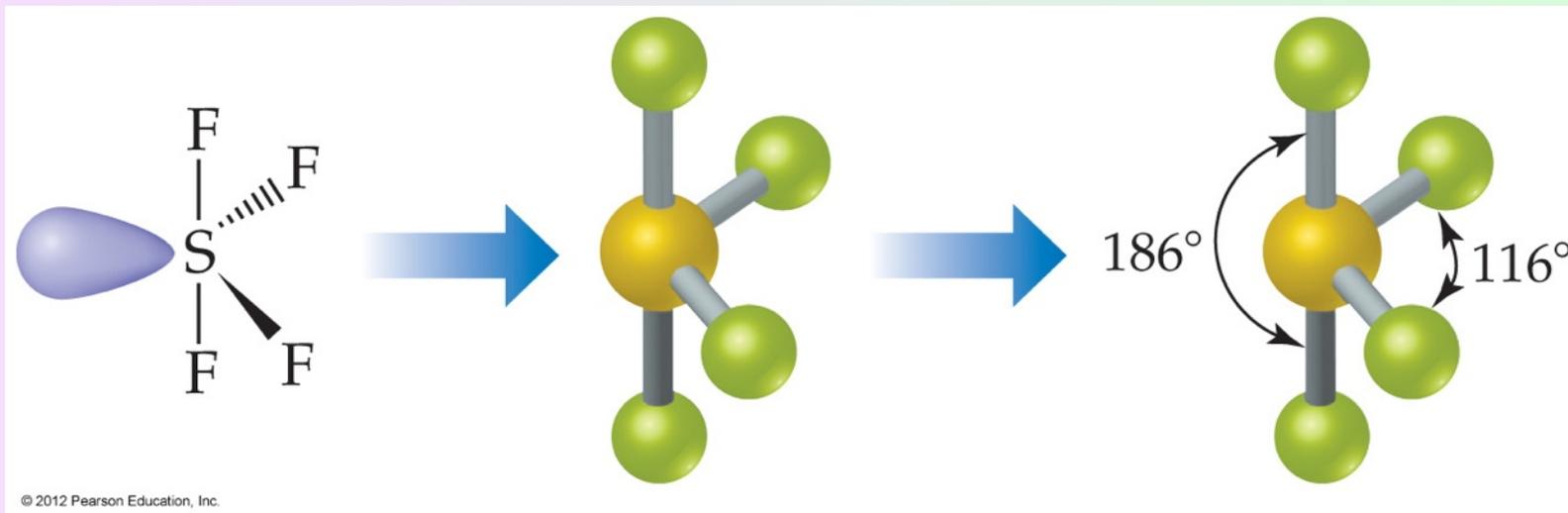
34 electrons

5 electron
pairs

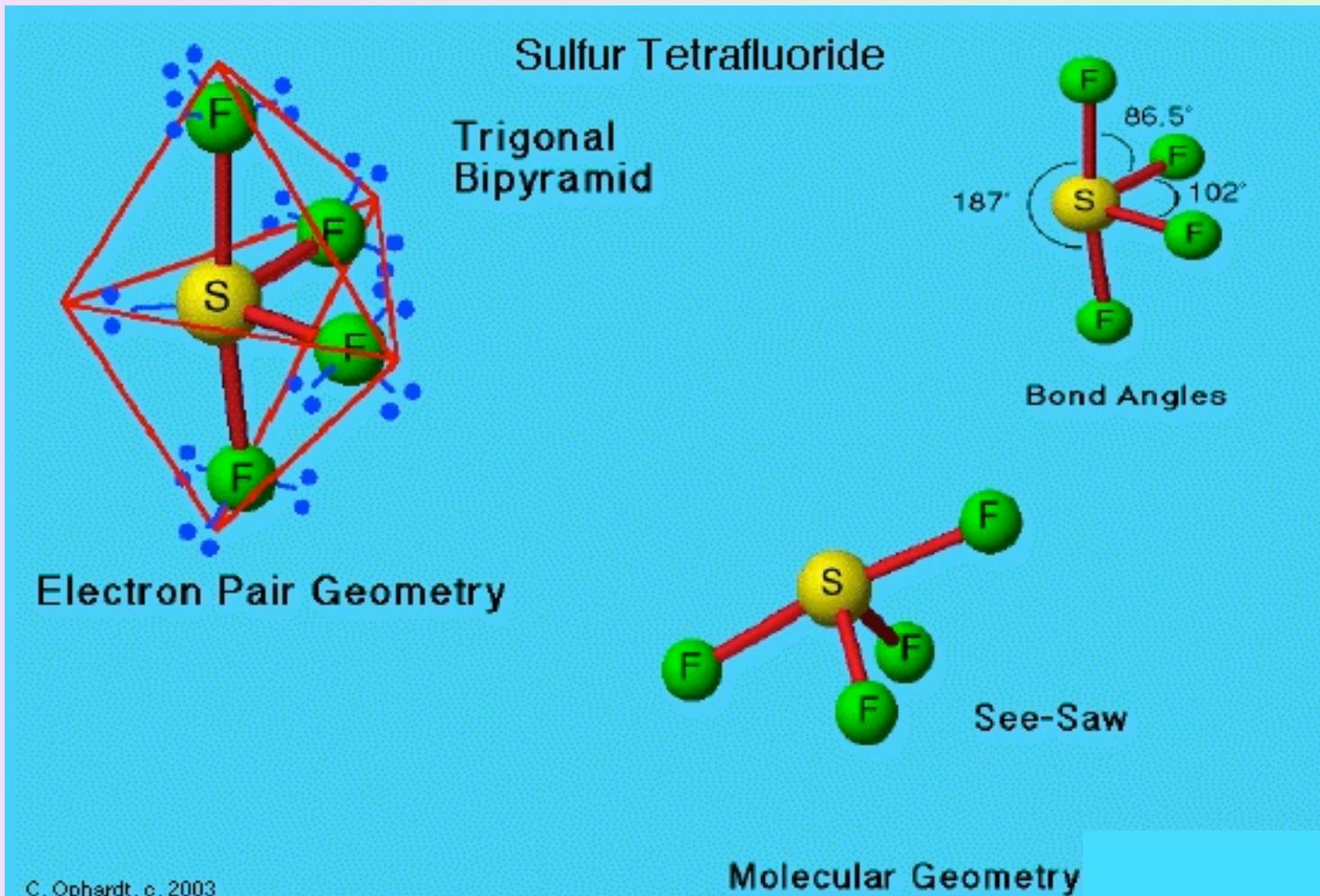


seesaw shaped;
trigonal bipyramidal
arrangement of electron pairs

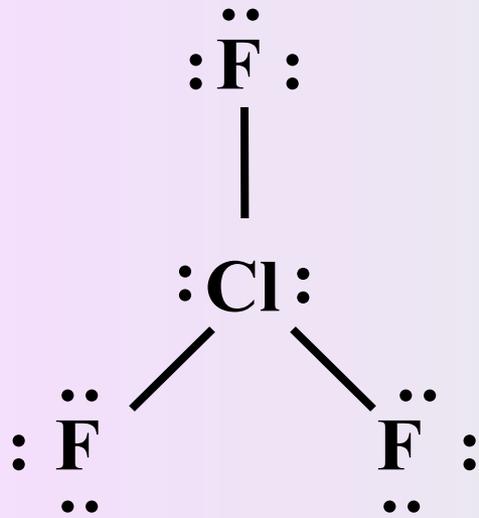
Sulfur tetrafluoride (SF₄)



Sulfur tetrafluoride (SF_4)

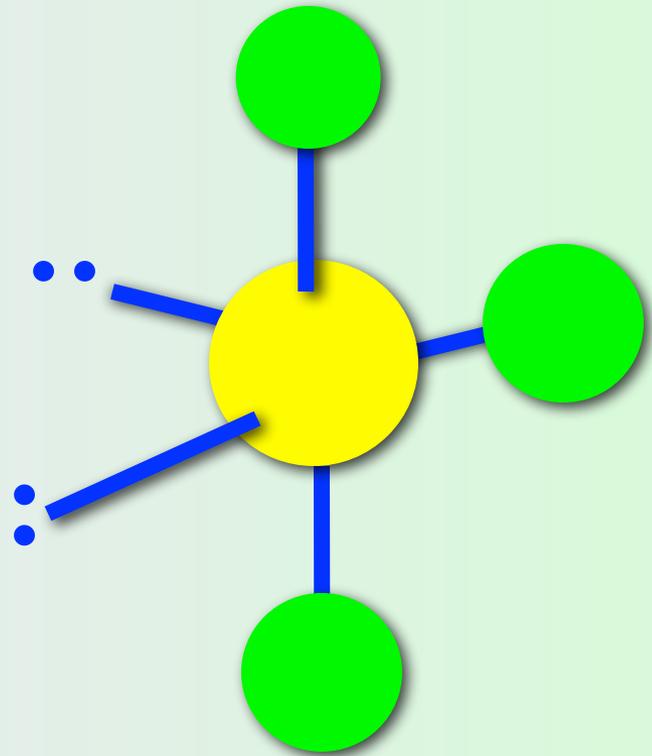


Chlorine trifluoride



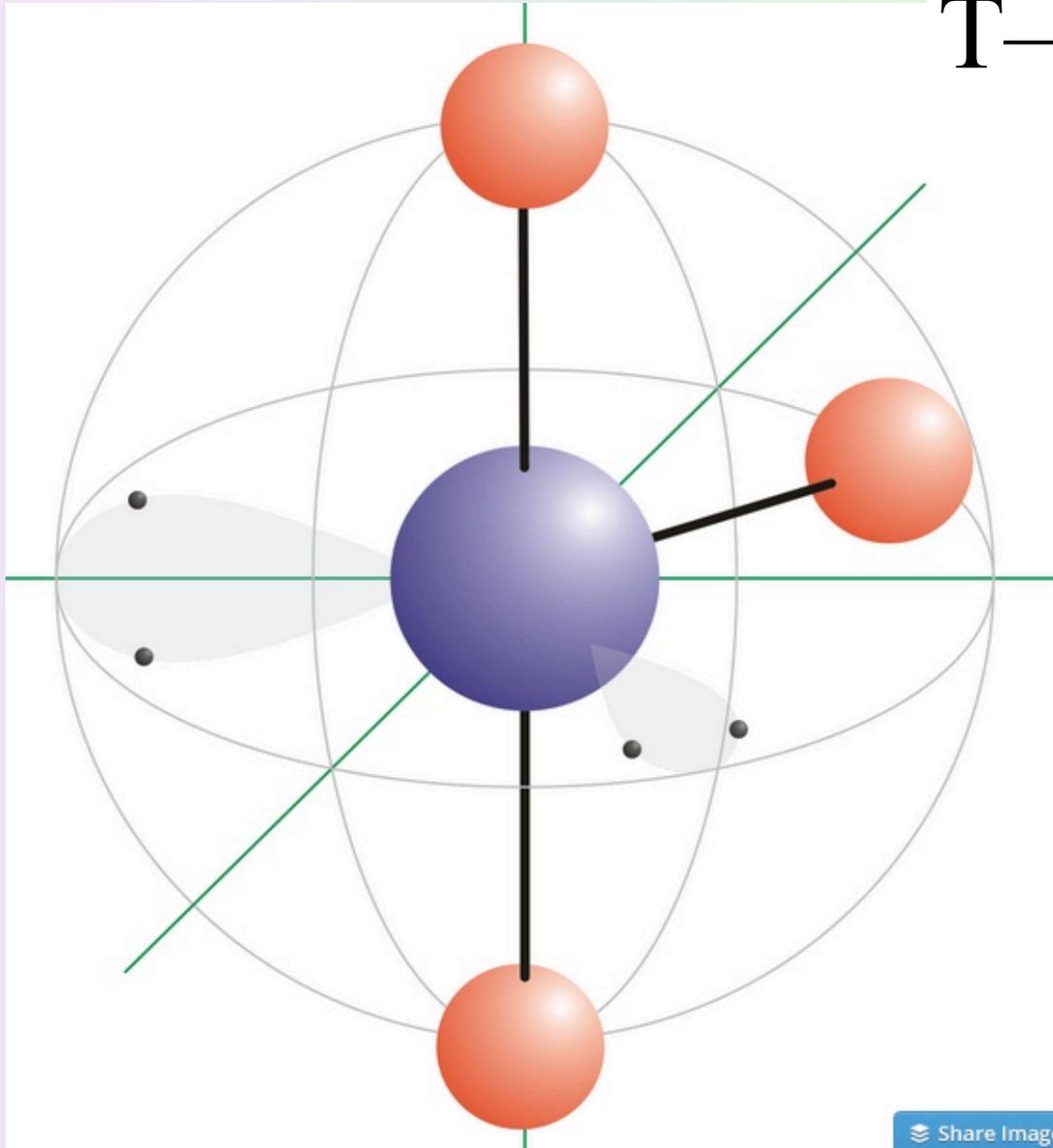
28 electrons

5 electron pairs



T-shaped

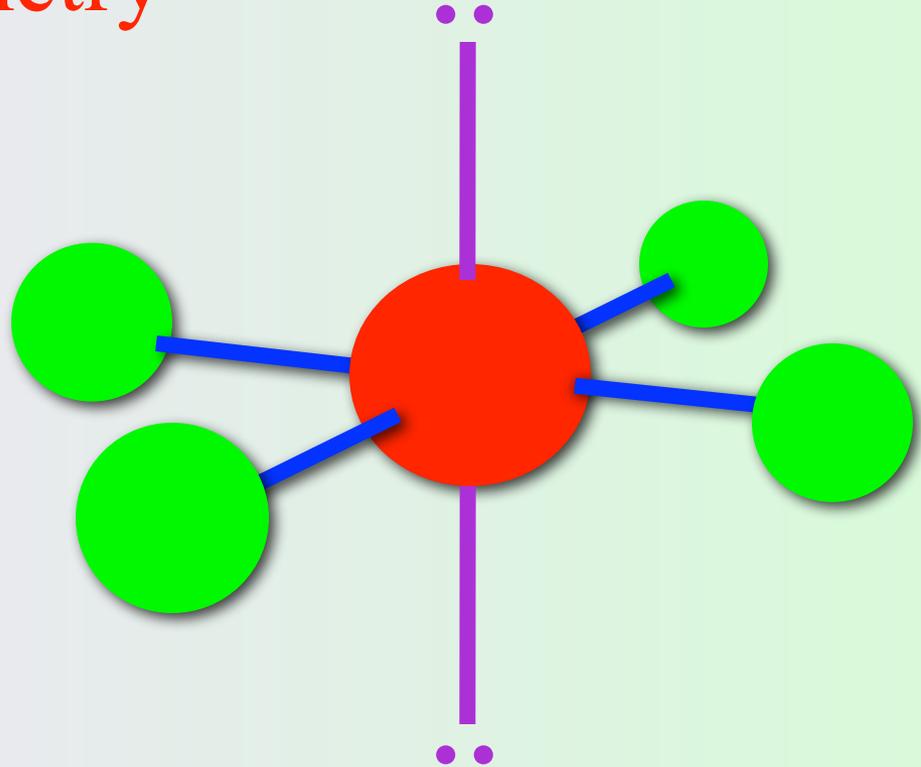
T-shaped



Xenon tetrafluoride

six electrons; octahedral arrangement of electron pairs

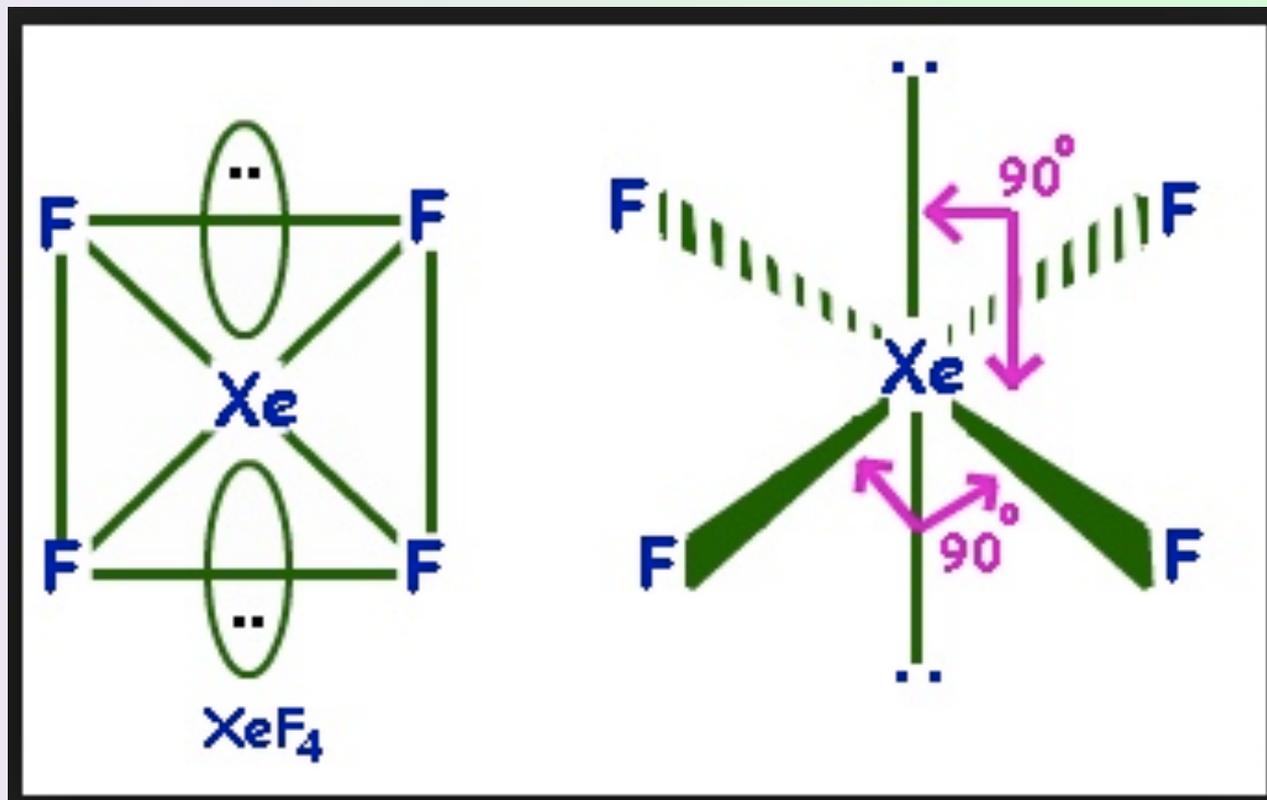
square planar geometry



Xenon tetrafluoride

six electrons; octahedral arrangement of electron pairs

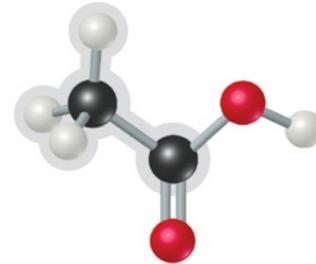
square planar geometry



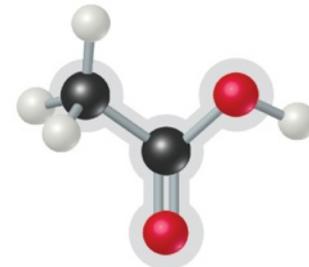
Geometry of Molecules with More Than One Central Atom

Larger Molecules

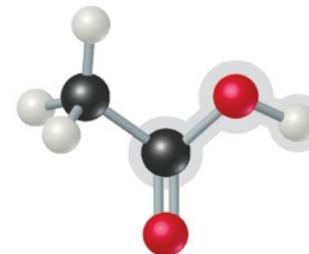
In larger molecules, it makes more sense to talk about the geometry about a particular atom rather than the geometry of the molecule as a whole.



Electron-domain geometry tetrahedral,
molecular geometry tetrahedral



Electron-domain geometry trigonal planar,
molecular geometry trigonal planar



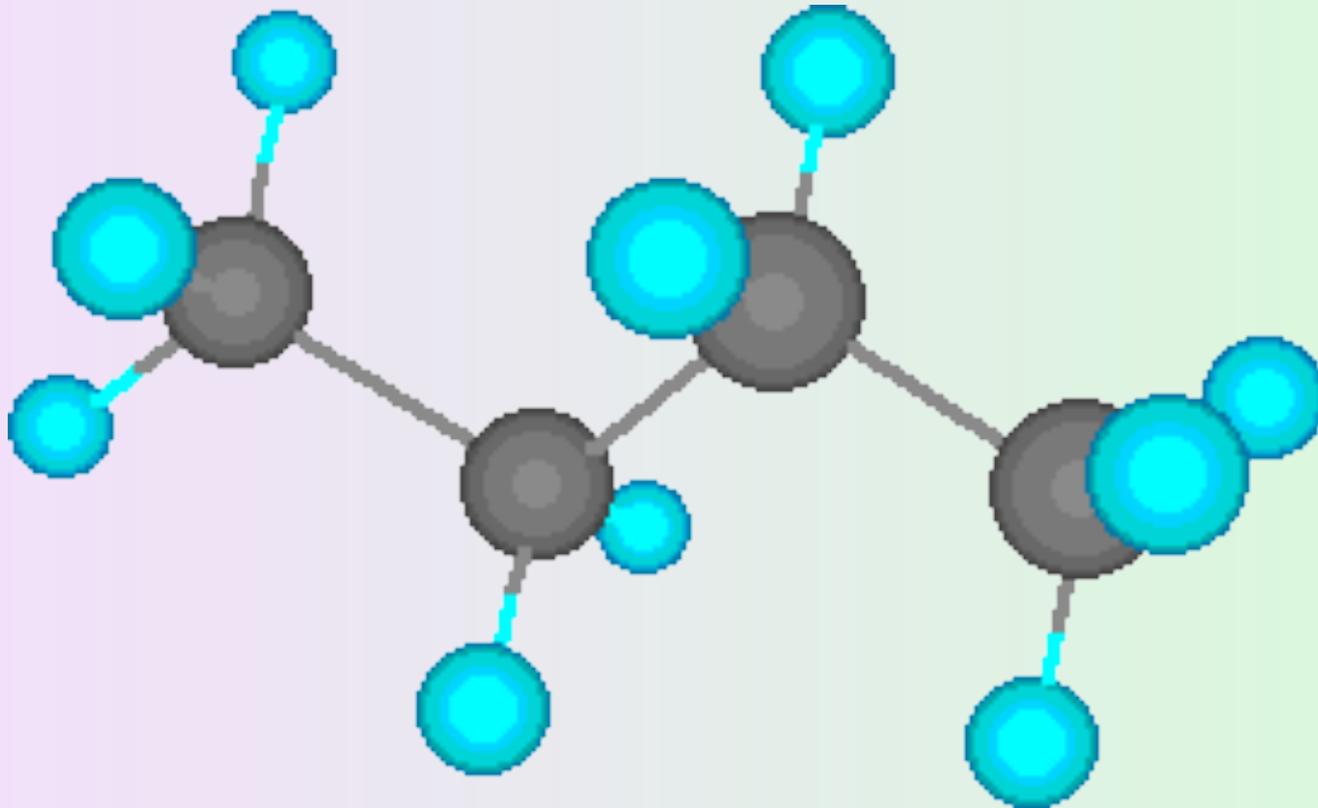
Electron-domain geometry tetrahedral,
molecular geometry bent

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Most molecules

lack a “central” atom

therefore, look for local stereochemistry



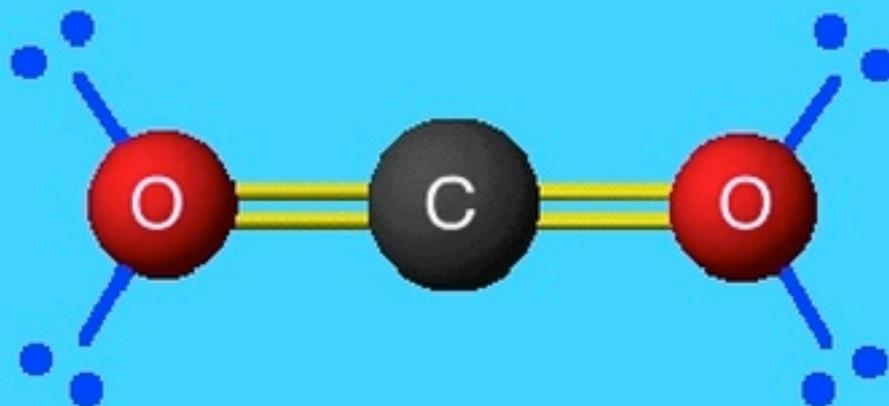
Guidelines for Applying the VSEPR Model

(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

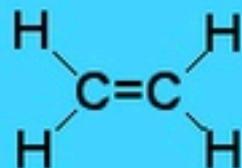


Linear

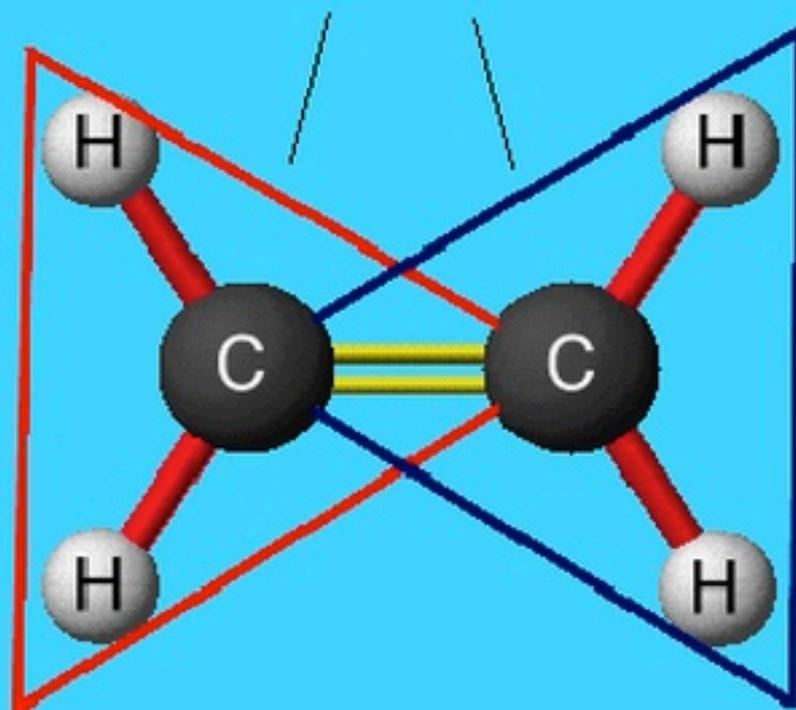


Electron Pair Geometry

Ethene or
Ethylene



Trigonal Planar



Molecular Geometry