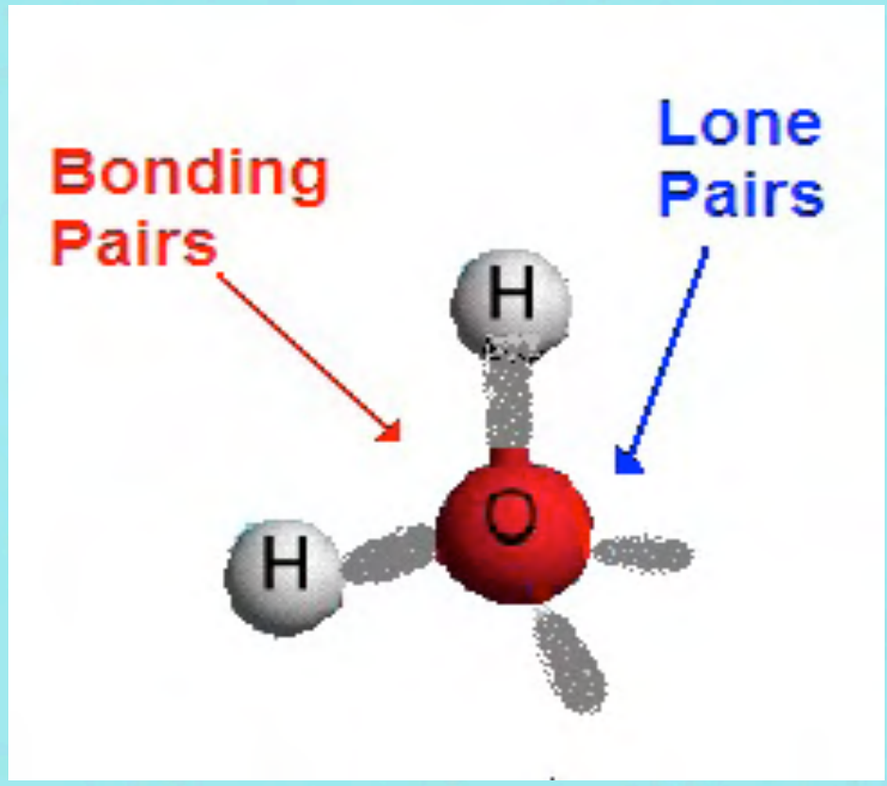
Structure & Properties

Predicting Molecular shape & VSEPR theory!

Valence Shell Electron Pair Repulsion

- When trying to determine the shape of a molecule, we must consider two things:
  - The electrons in bonds (bond pairs)
  - The electrons not in bonds (lone pairs)



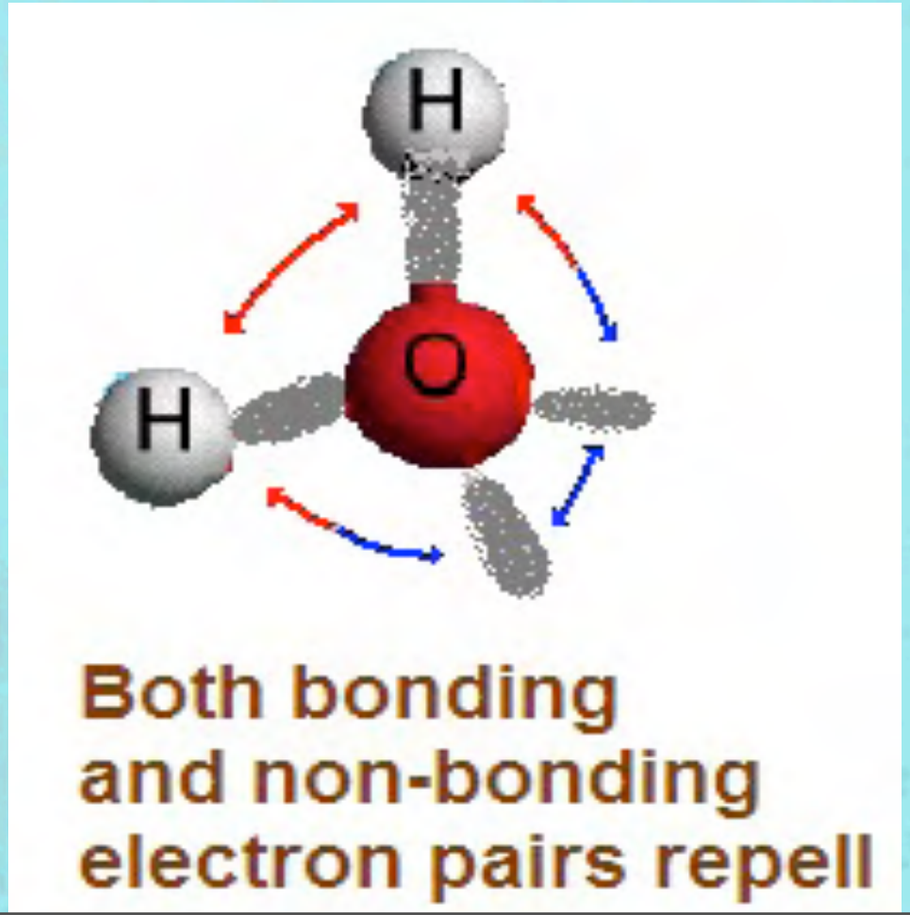
- <u>REMEMBER!</u> Electrons are negatively charged and will repel each other.

VSEPR

- Valence Shell Electron Pair Repulsion (VSEPR) theory can be used to predict the geometric shapes of molecules.
- VSEPR revolves around the principle that electrons repel each other.
- One can predict the shape of a molecule by finding a pattern where electron pairs are as far from each other as possible.

VSEPR

- Molecules will be shaped in a way in order to minimize contact between electrons
- Lone pair (those not in a bond) electrons cause the most repelling since they take up so much space
- In order of severity of repelling:
  - Lone Pair -Lone Pair
  - Lone Pair -Bond Pair
  - Bond Pair- Bond Pair



Exceptions

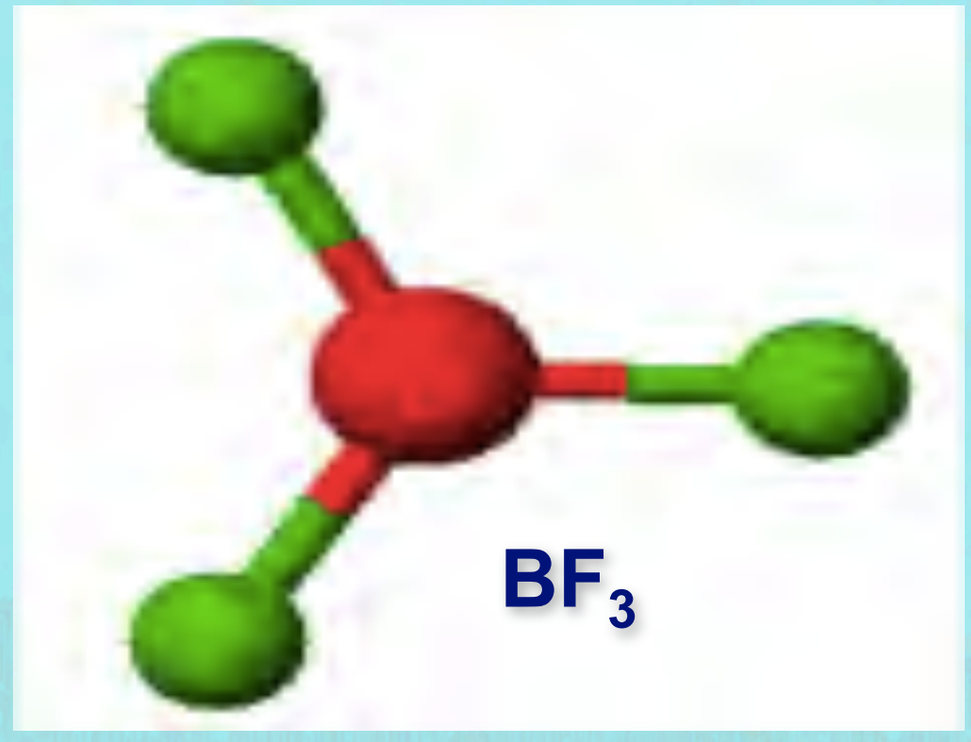
- Violations of the octet rule usually occur with B and elements of higher periods.
- Some common examples include: Be, B, P, S, and Xe.
- Be: 4

B: 6

P: 8 OR 10

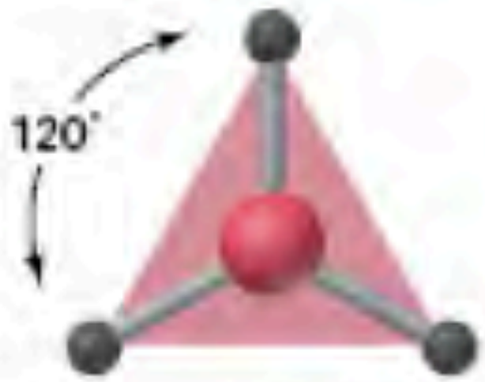
S: 8, 10, OR 12

Xe: 8, 10, OR 12

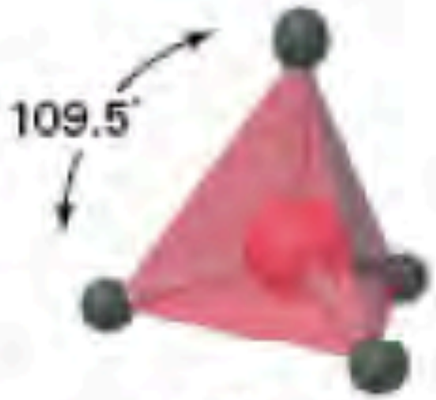


5 Basic Shapes

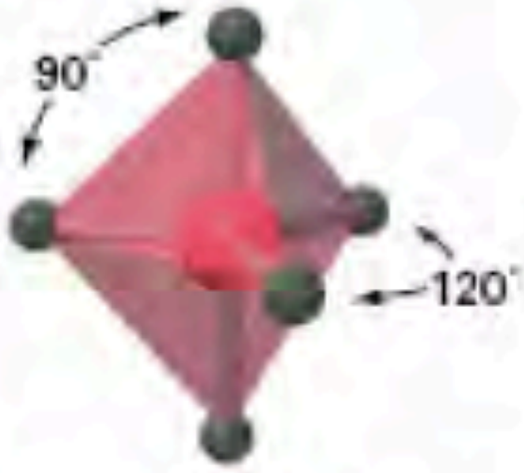
linear



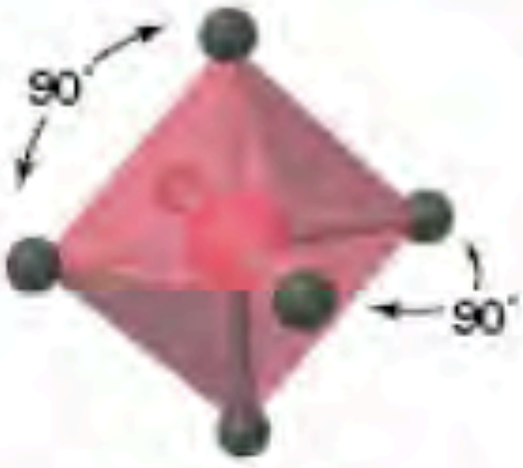
trigonal planar



tetrahedral



trigonal bipyramidal



octahedral

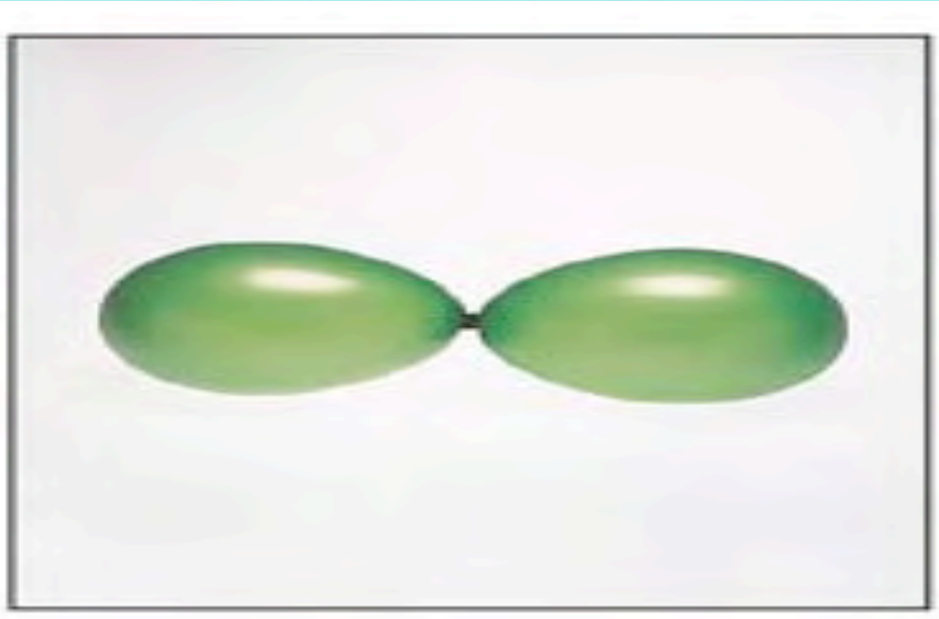
ure 4.11 **The five basic electron-group arrangements and their bond angles**

Notation

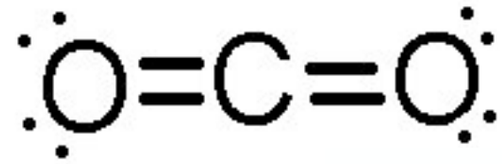
- Start by drawing the Lewis Structure. Then assign A, X, E
- A represents the central atom
- X represents the number of bonds to the central atom
- E represents the number of lone pair electrons on the central atom
- ie) AX_4, AX_2E_2, AX_2

Linear

- ie) CO_2
- 2 attachments, no lone pairs (AX_2)
- 180 degrees between atoms

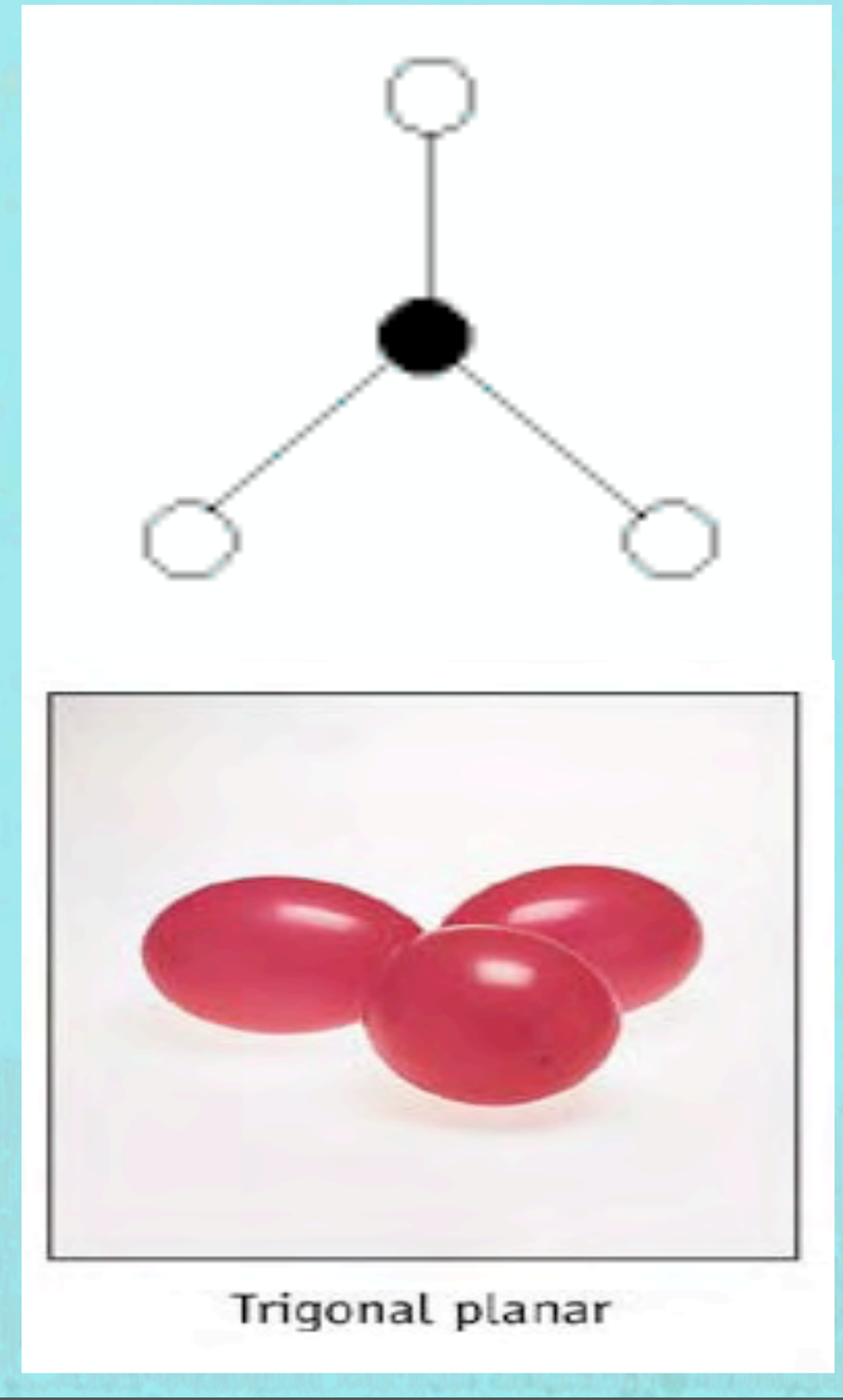


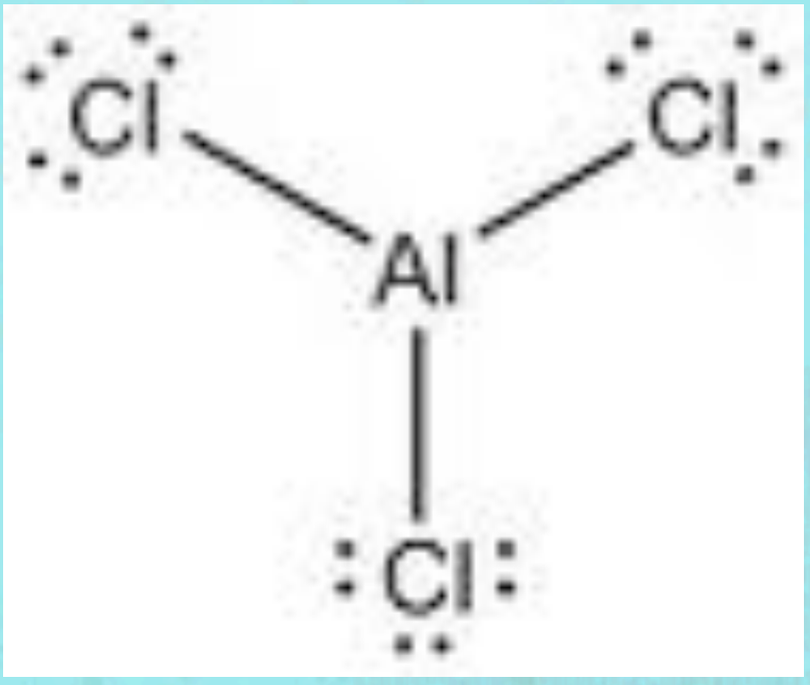
Linear



Trigonal Planar

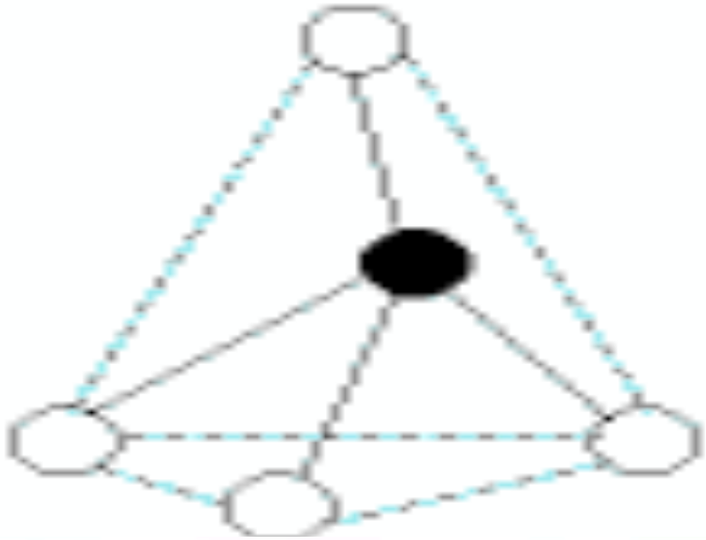
- ie) $AlCl_3$
- 3 attachments, no lone pairs (AX_3)
- Bonds are flat, 120 degrees apart





Tetrahedral

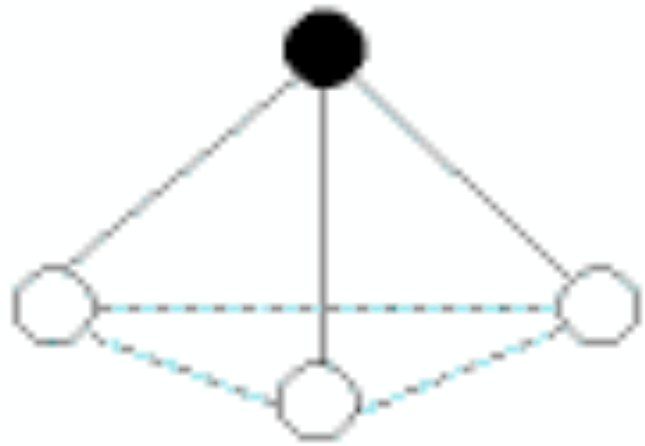
- ie) CH_4
- 4 attachments, no lone pairs (AX_4)
- 109.5 degrees

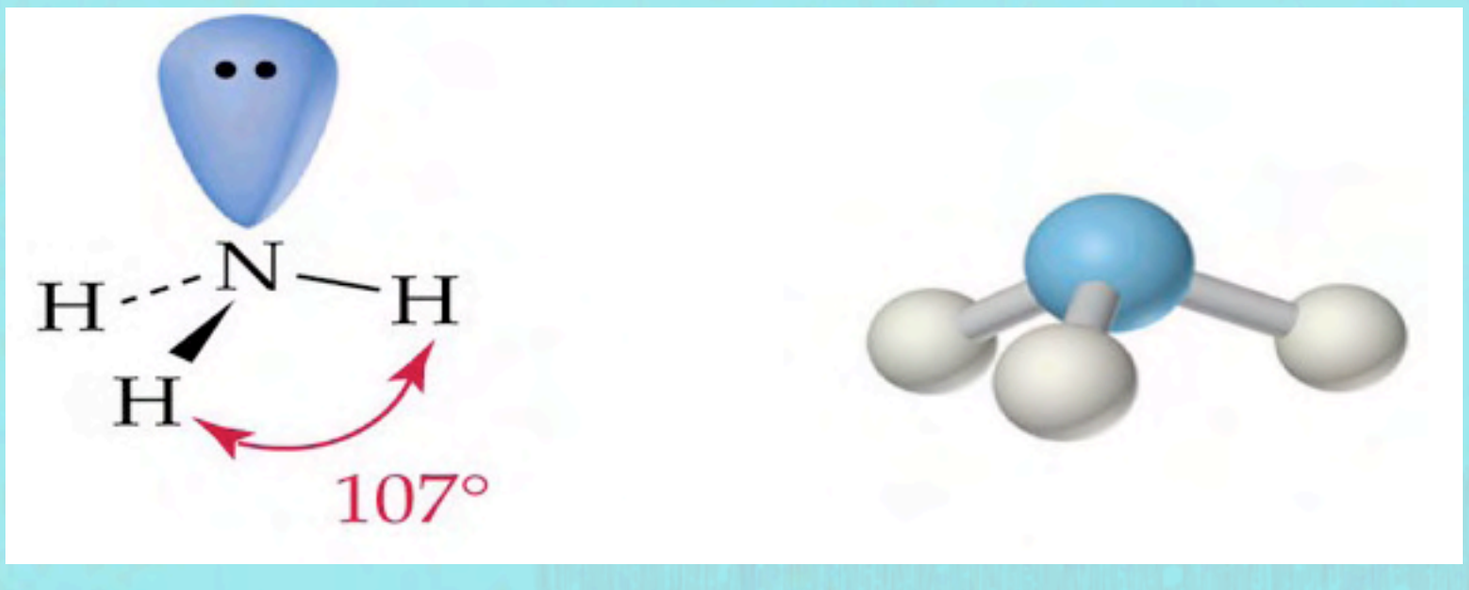


Tetrahedral

Tetrahedral: Trigonal Pyramidal

- ie) NH_3
- 4 attachments total, 1 of which is a lone pair
- AX_3E_1



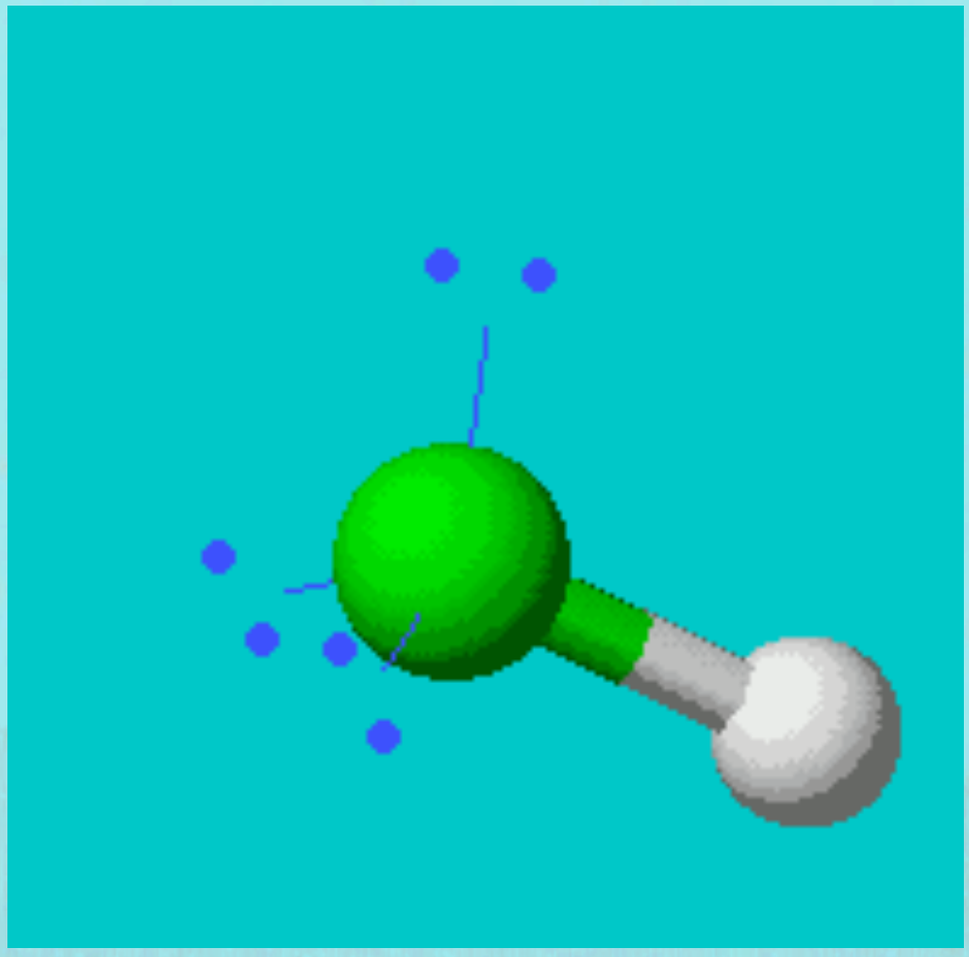


Tetrahedral: Bent

- ie) H_2O
- 4 attachments total, 2 of which are lone pairs
- AX_2E_2

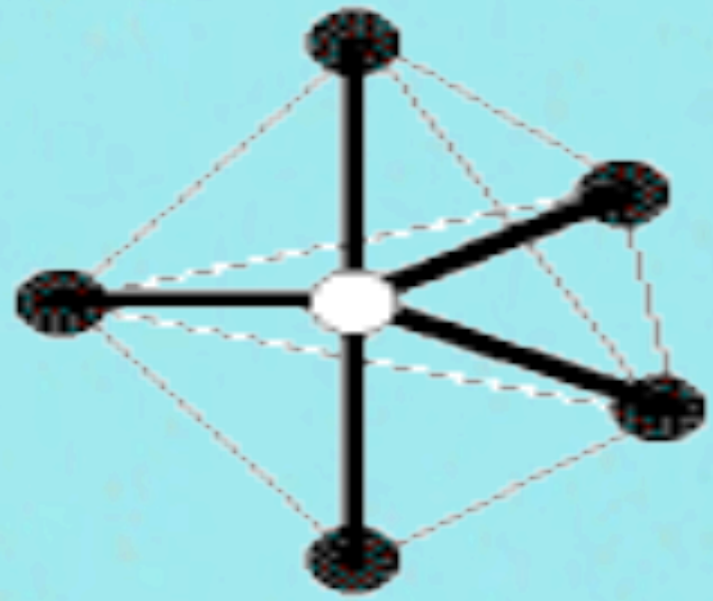
Another Linear!

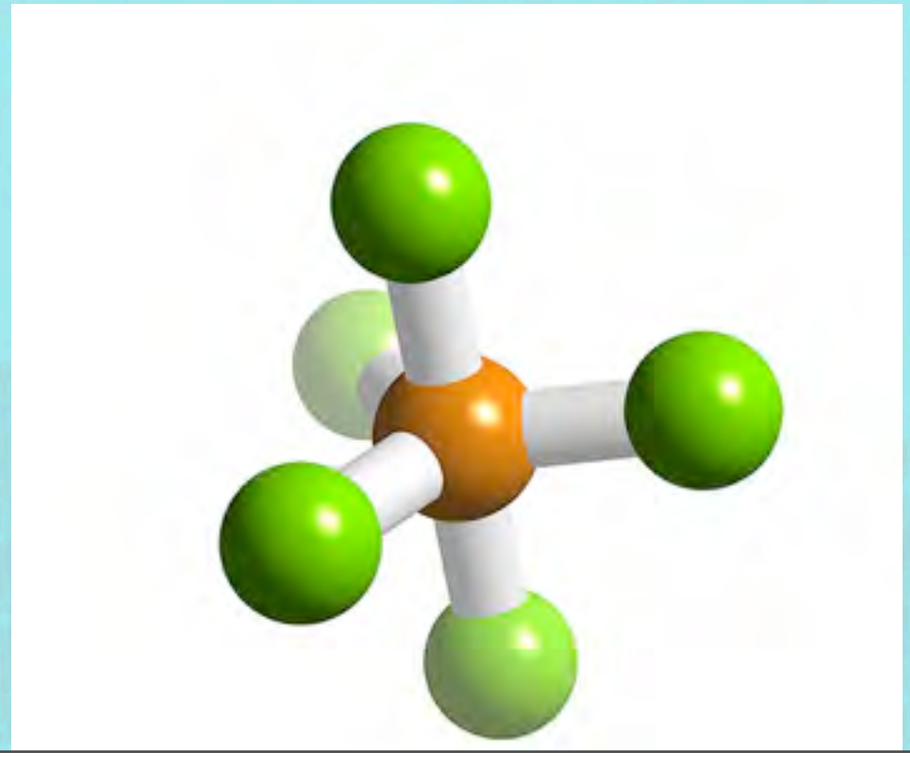
- ie) HF
- 4 attachments, 3 of which are lone pairs
- AXE_4



Trigonal Bipyramidal

- ie) PCl_5
- 5 attachments, no lone pairs
- AX_5
- 120 degrees, at 90 degrees to each other



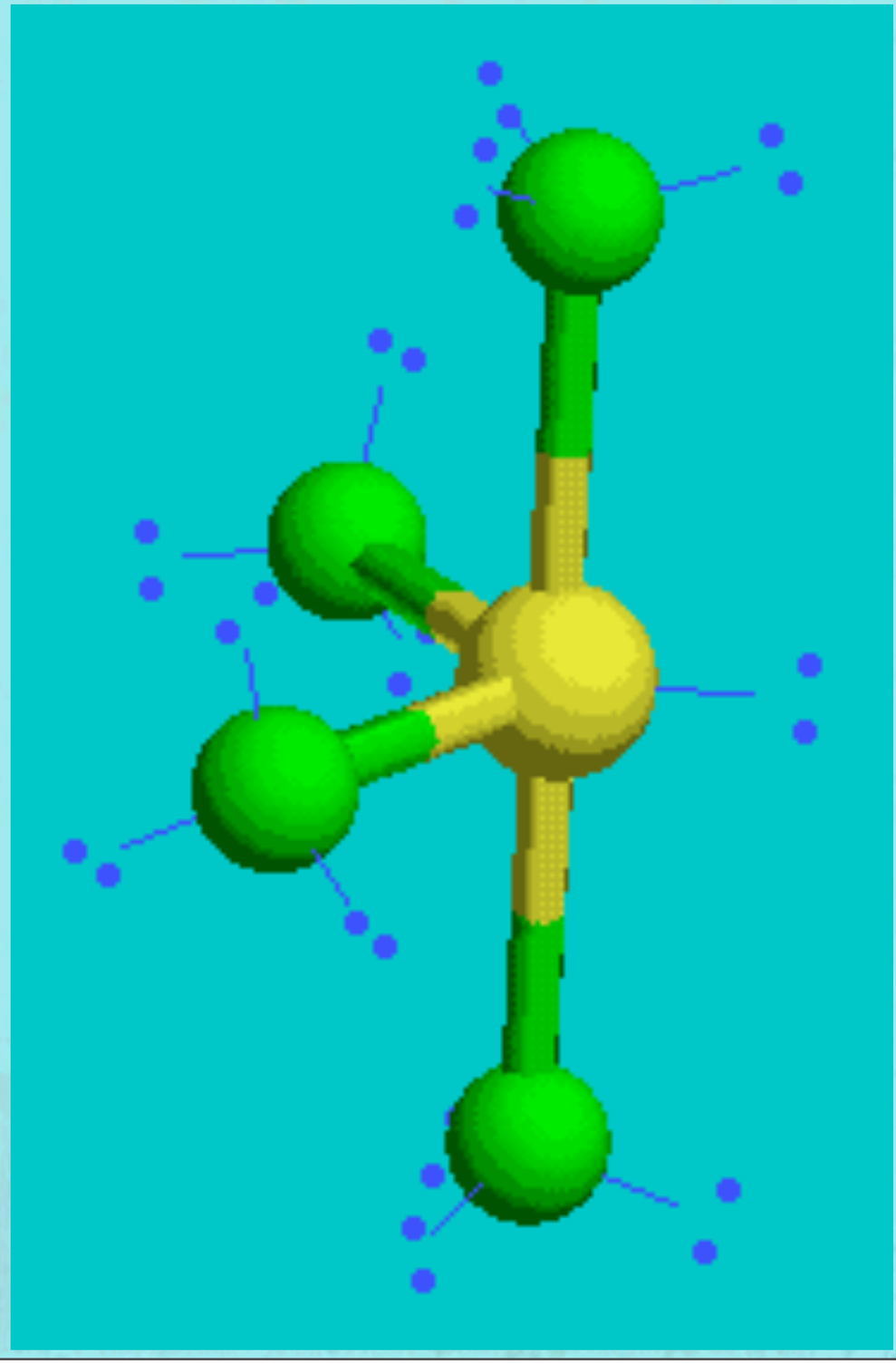


Trigonal Bipyramidal: SeeSaw

- ie) SF_4

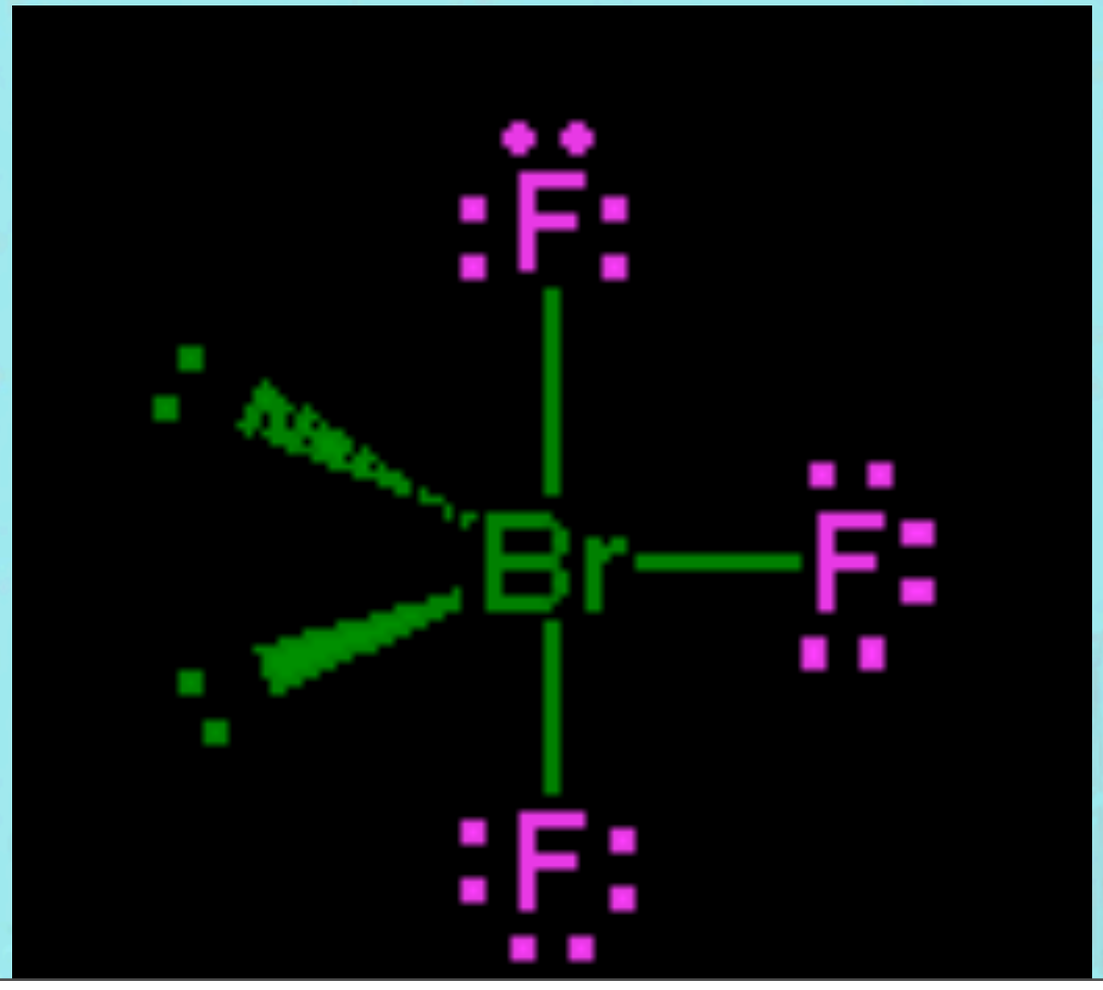
- 5 attachments, 1 of which is a lone pair

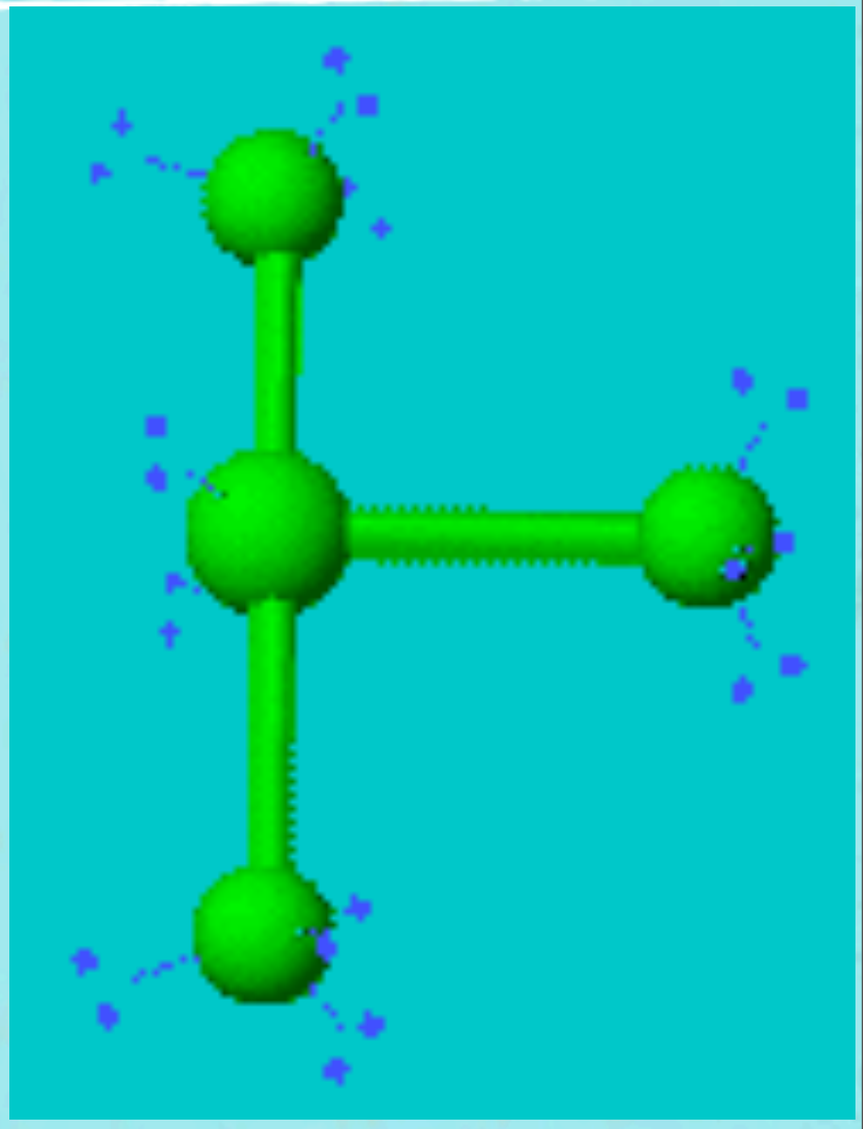
- AX_4E_1



Trigonal Bipyramidal: T-Shaped

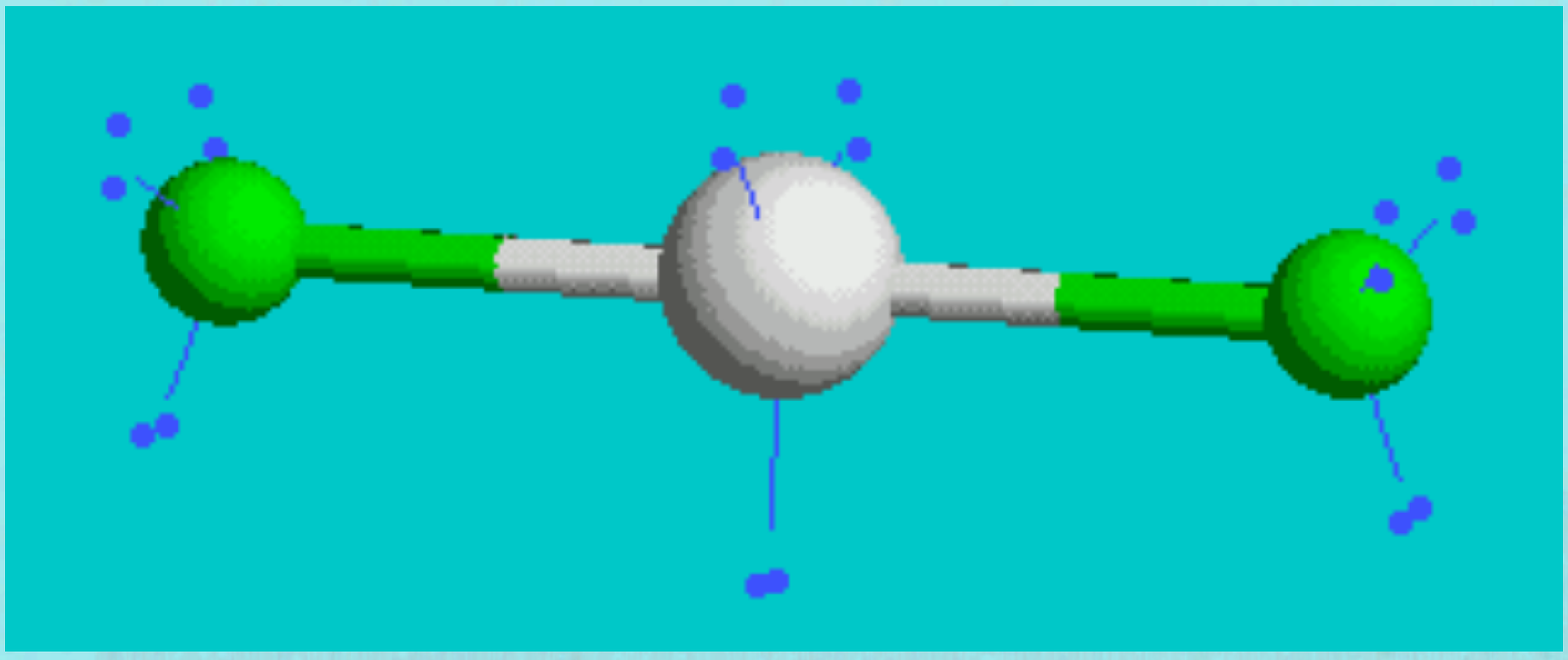
- ie) BrF_3
- 5 attachments, 2 of which are lone pairs
- AX_3E_2
- T-shaped





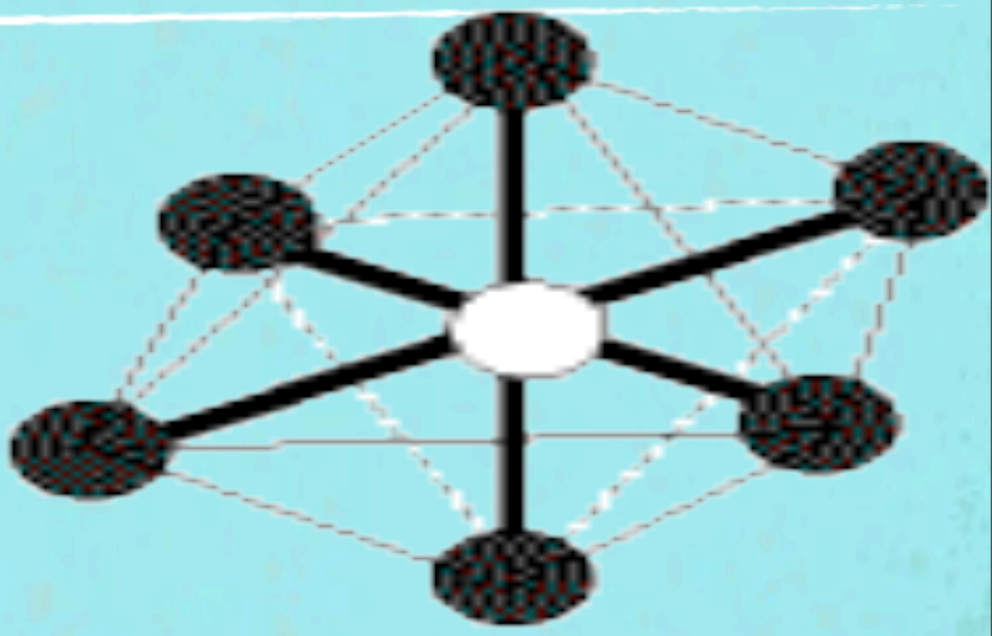
One more Linear!

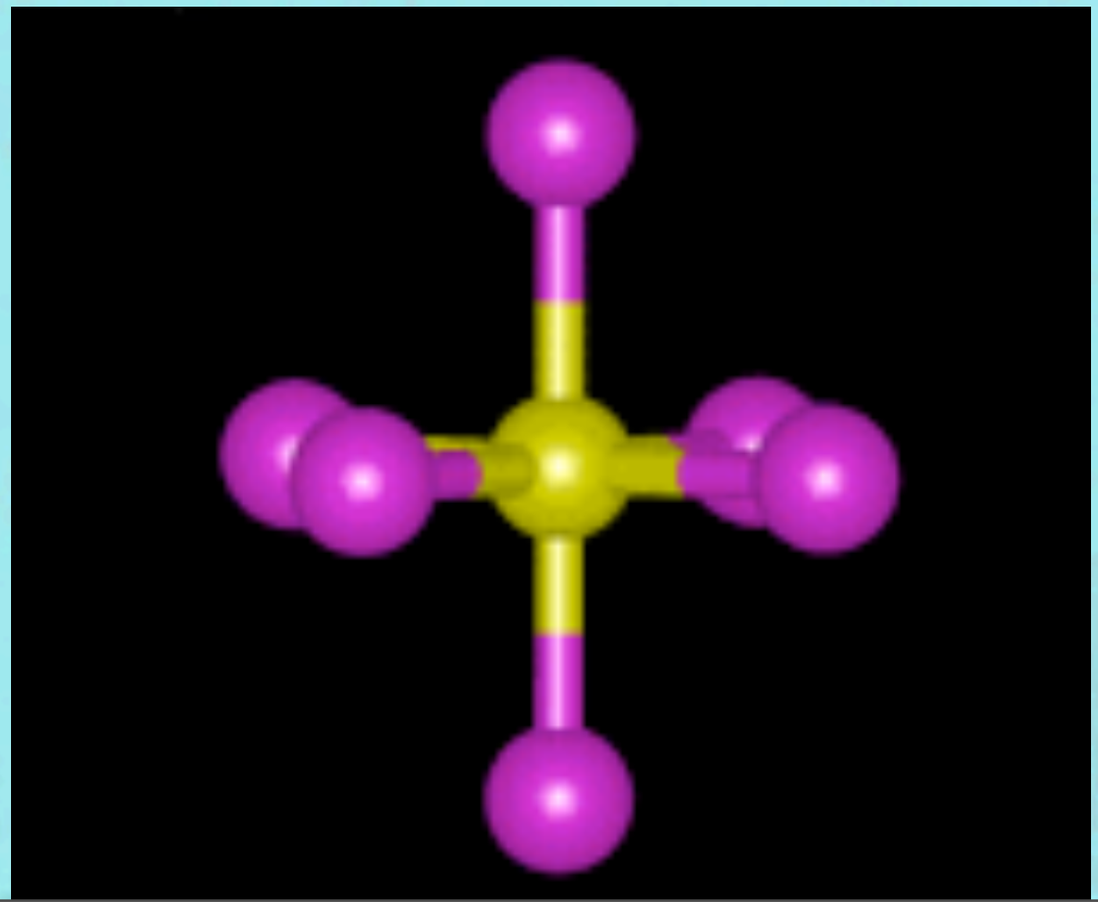
- ie) XeF_2
- 5 attachments, 3 of which are lone pairs!
- AX_2E_3
- 180 degrees to each other, with the lone pairs above/below plane



Octahedral

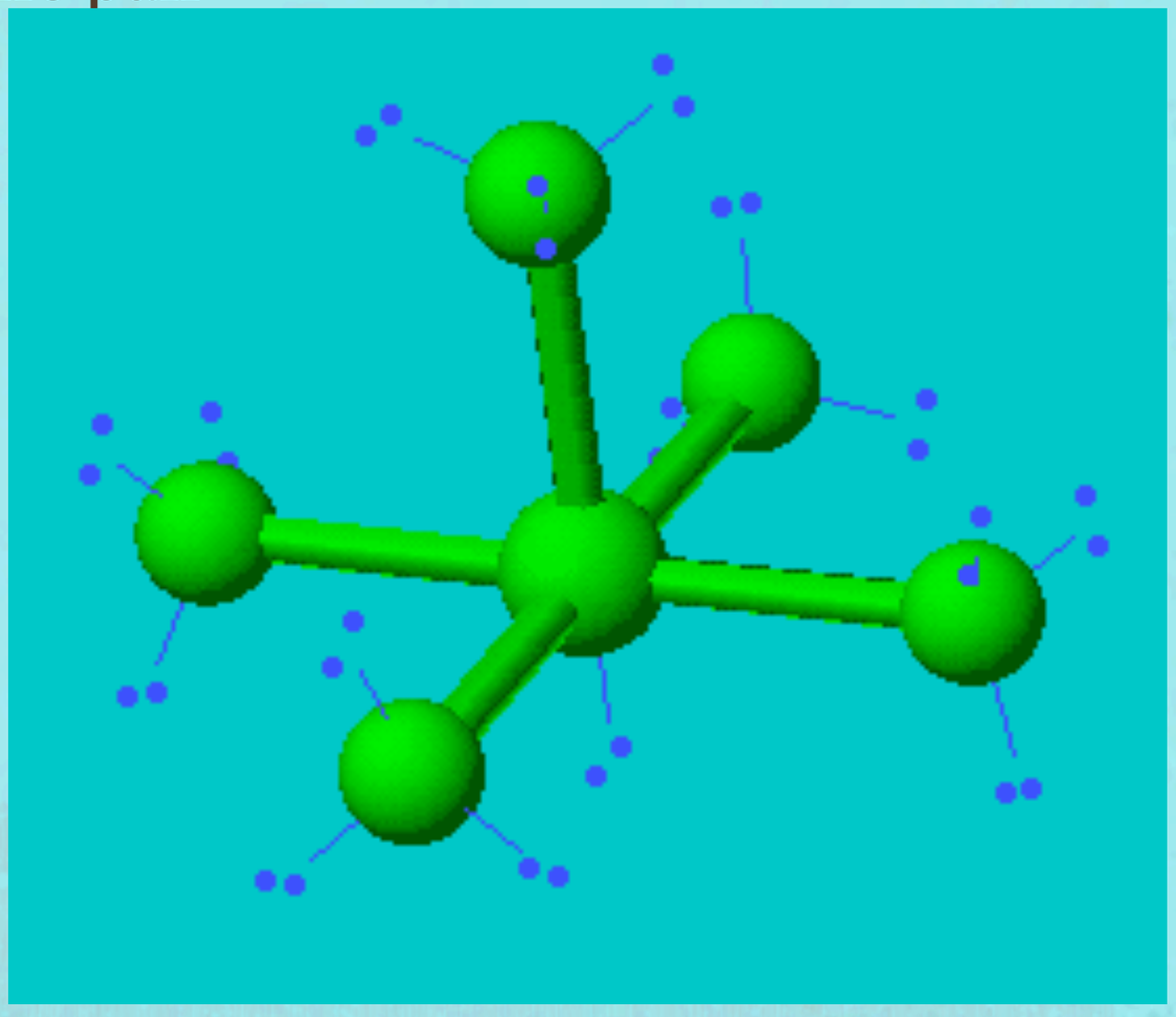
- ie) SF_6
- 6 attachments
- AX_6
- Bonds are all 90 degrees to each other





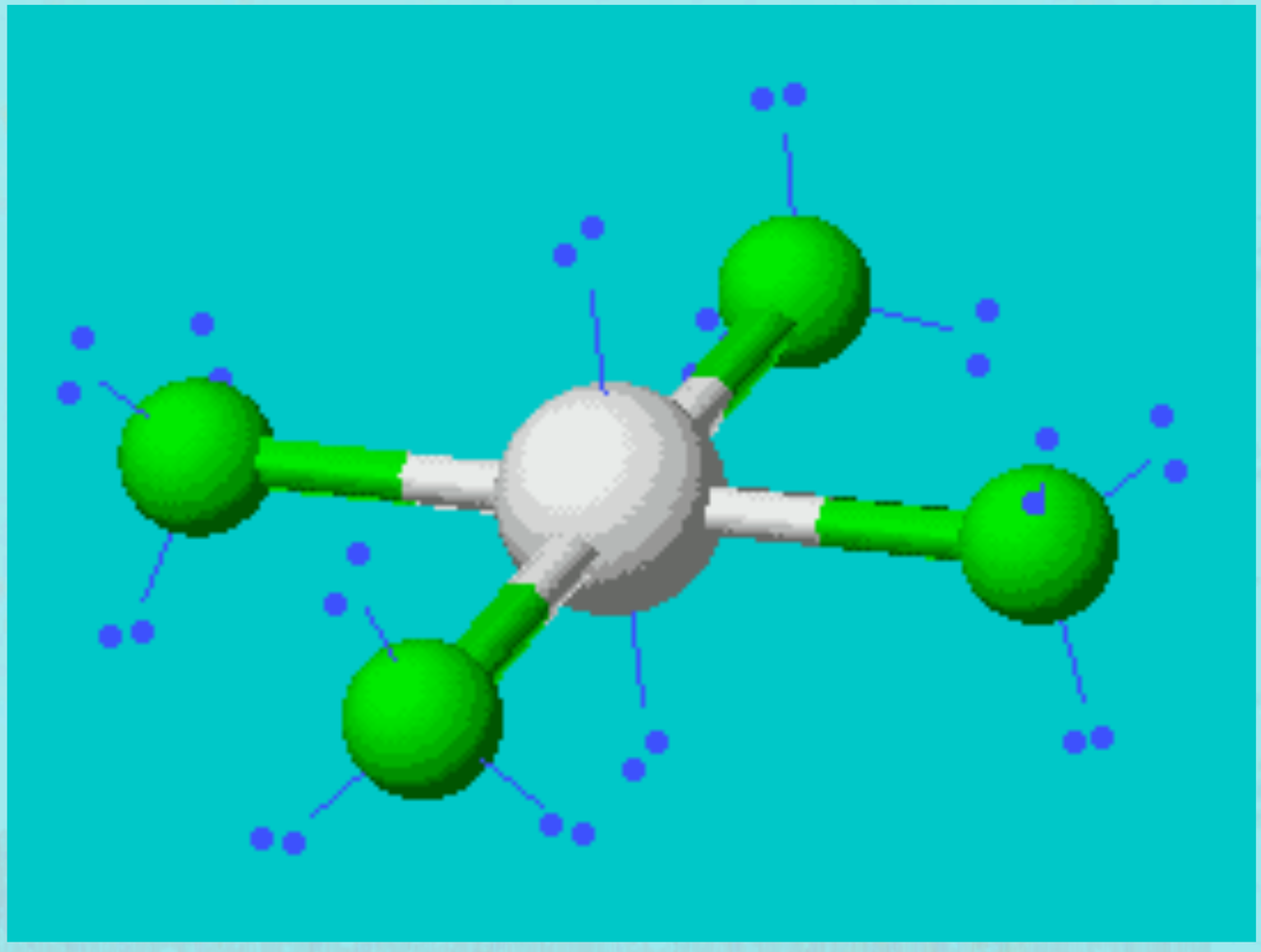
Square Pyramidal

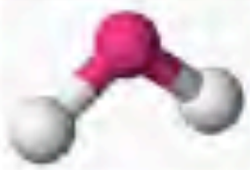
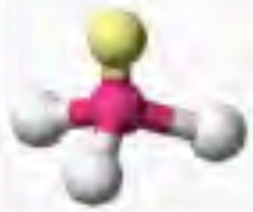
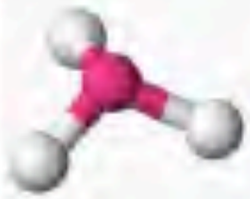
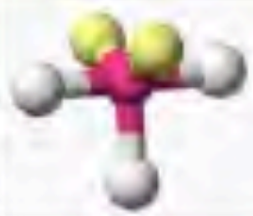
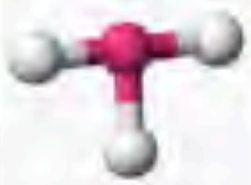
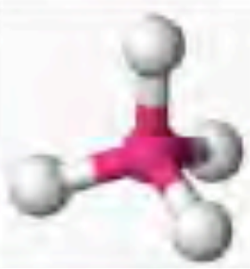
- ie) ClF_5
- 6 attachments, 1 of which is a lone pair
- AX_5E_1
- 90 degrees, 1 atom above plane

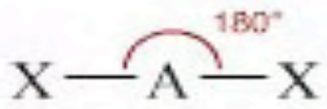


Square Planar

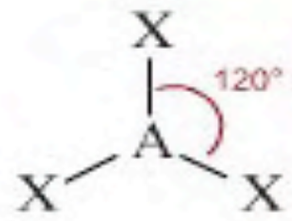
- ie) XeF_4
- 6 attachments, 2 lone pairs
- AX_4E_2
- 90 degrees in a plane
- Lone pairs above/below



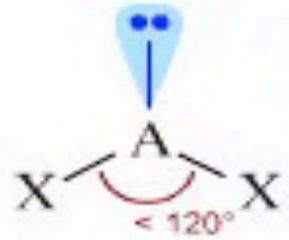
Molecule Type	Shape	Electron arrangement[†]	Geometry[‡]	Examples
AX_1E_n	Diatomic			HF, O_2
AX_2E_0	Linear			$BeCl_2$, $HgCl_2$, CO_2
AX_2E_1	Bent			NO_2^-, SO_2, O_3
AX_2E_2	Bent			H_2O, OF_2
AX_2E_3	Linear			XeF_2, I_3^-
AX_3E_0	Trigonal planar			BF_3, CO_3^{2-}, NO_3^-, SO_3
AX_3E_1	Trigonal pyramidal			NH_3, PCl_3
AX_3E_2	T-shaped			ClF_3, BrF_3
AX_4E_0	Tetrahedral			CH_4, PO_4^{3-}, SO_4^{2-}, ClO_4^-



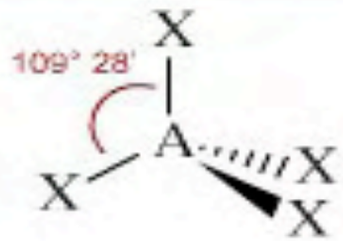
AX_2
Linear



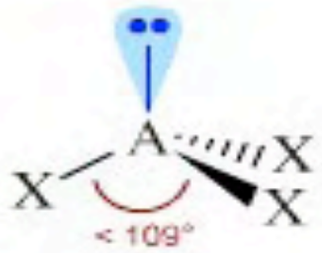
AX_3
Trigonal planar



AX_2E_1
Bent or Angular

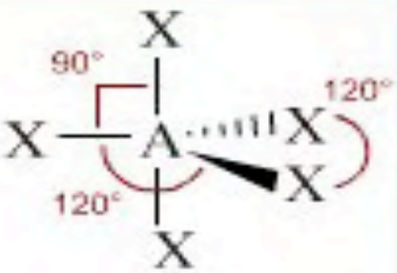


AX_4
Tetrahedral

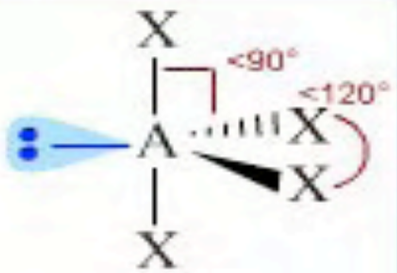


AX_3E_1
Trigonal pyramidal

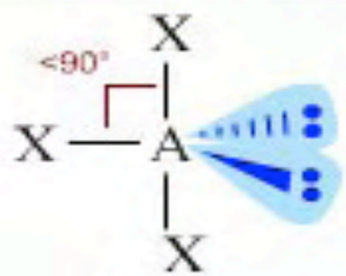
AX_2E_2
Bent or Angular



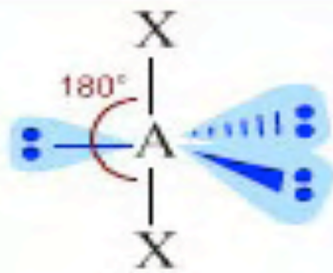
AX_5
Trigonal bipyramidal



AX_4E_1
Sawhorse or Seesaw

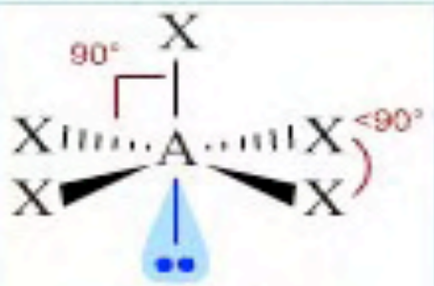


AX_3E_2
T-shape

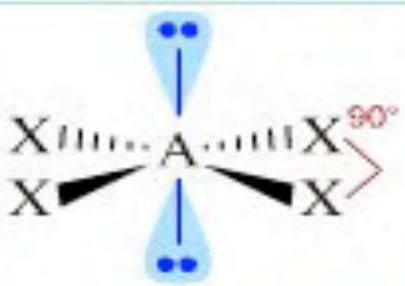


AX_2E_3
Linear

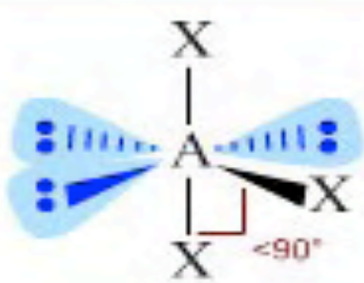
AX_6
Octahedral



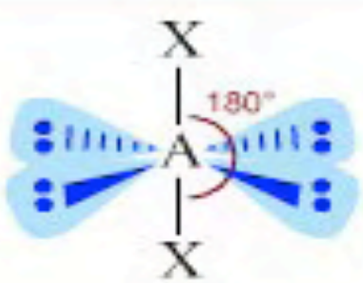
AX_5E_1
Square pyramidal



AX_4E_2
Square planar



AX_3E_3
T-shape



AX_2E_4
Linear

Draw Lewis structures & predict shape

- HCN
- SO_3
- Cl_2CO
- SO_2
- O_3

- XeO_3
- PF_5
- SF_4
- BrF_3
- SF_6
- BrF_5
- IO_4^-