Chem 111

Lecture 29

Announcement

- None

Experience a NEW way of teaching science

"Bhopal Disaster: A Case Study"

An Exciting Workshop Presented by iCons Faculty

WHO: Majors from College of Natural Science and College of Engineering
WHEN: Thursday, Nov. 18 6:30-8:00 PM
OR
Tuesday, Nov. 23 6:30 – 8:00 PM
WHY: Because YOU can make a difference

Integrated Concentration in Science

- **Free Pizza**
- **Space is limited!**

Register Now by Email:
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Homework

- Continue Reading Chapter 8
- Owl Homework

Recap

A-A A=A

- Multiple Bonds ← A=A
- Lewis Structures
- Isoelectronic Species

same e^- valence

Formal Charge

A form of bookkeeping, used to determine charge assigned to an atom in a molecule.

The formal charge of an atom equals the number of valence electrons in the isolated atom, minus the number of assigned to the atom in the Lewis Structure.

1. All of the unshared (non-bonding) electrons are assigned to the atom on which they are found.

2. Half of the bonding electrons are assigned to each atom in the bond.

FC = Group Number – [Lone Pair e^- + ½ Bond Pair e^-]

Formal Charge

FC = Group Number – [Lone Pair e⁻ + ½ Bond Pair e⁻]

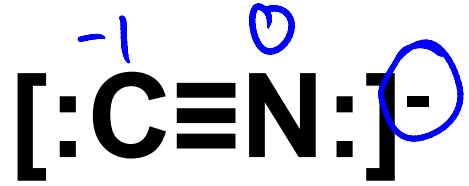
valance e⁻

C = 4 − (2 + 3)

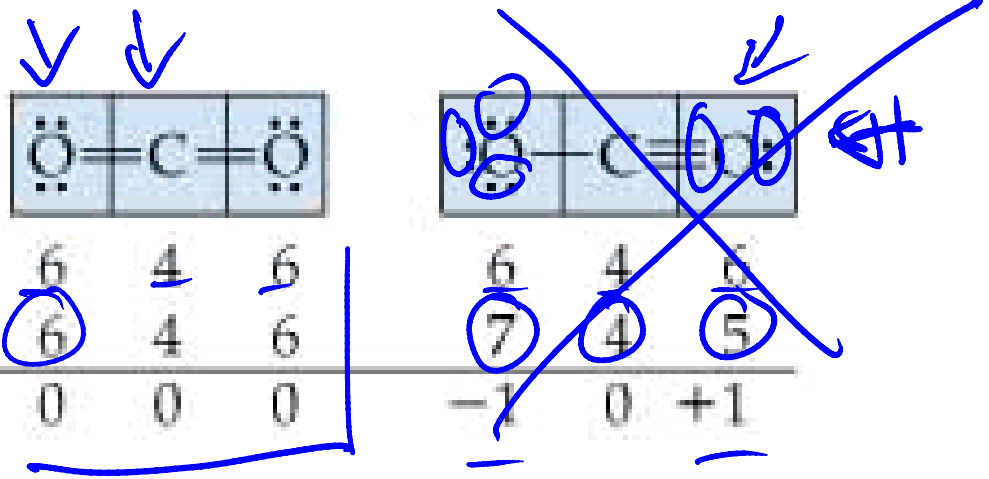
C = −1

N = 5 − [2 + 3)

N = 0



Some of the formal charges will equal will equal the overall charge of the molecule.

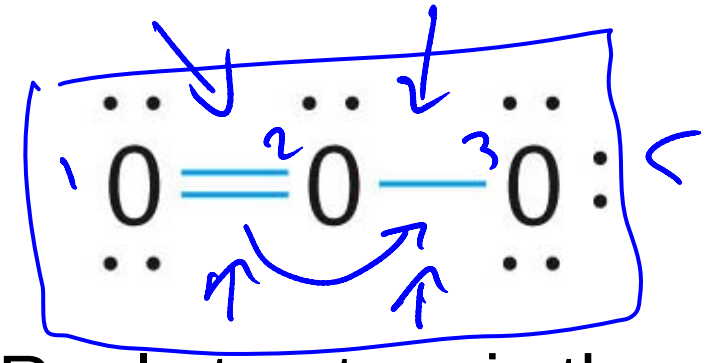


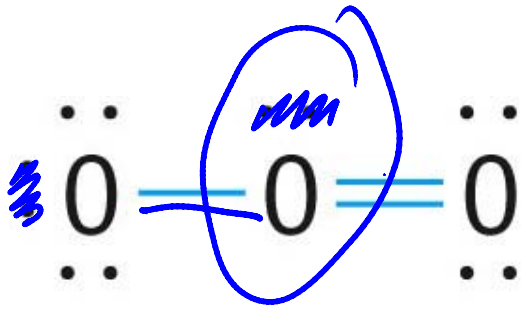
→ valence e⁻:	6	4	6	6	4	6
−(e⁻ assigned to atom):	6	4	6	7	4	5
formal charge:	0	0	0	−1	0	+1

When several Lewis structures are possible, the more stable ones are the ones that bear the smallest formal charges.

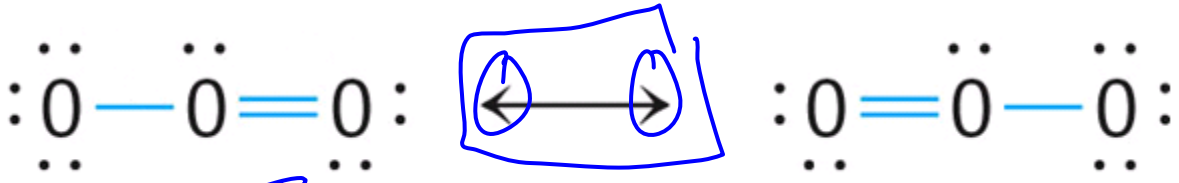
Resonance Structure

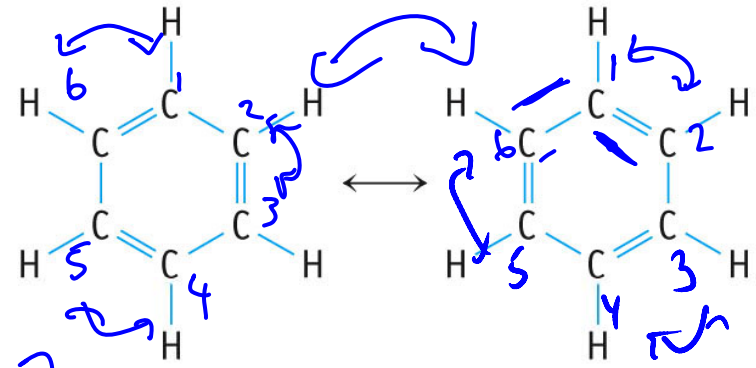
Consider O_3



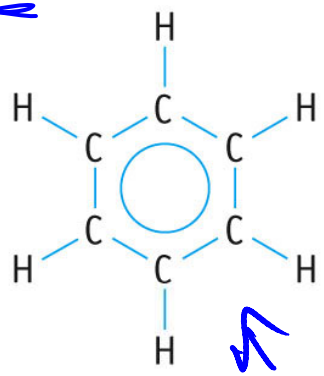


Real structure is the average of the two:





Resonance structures of benzene, C_6H_6



Abbreviated representation of

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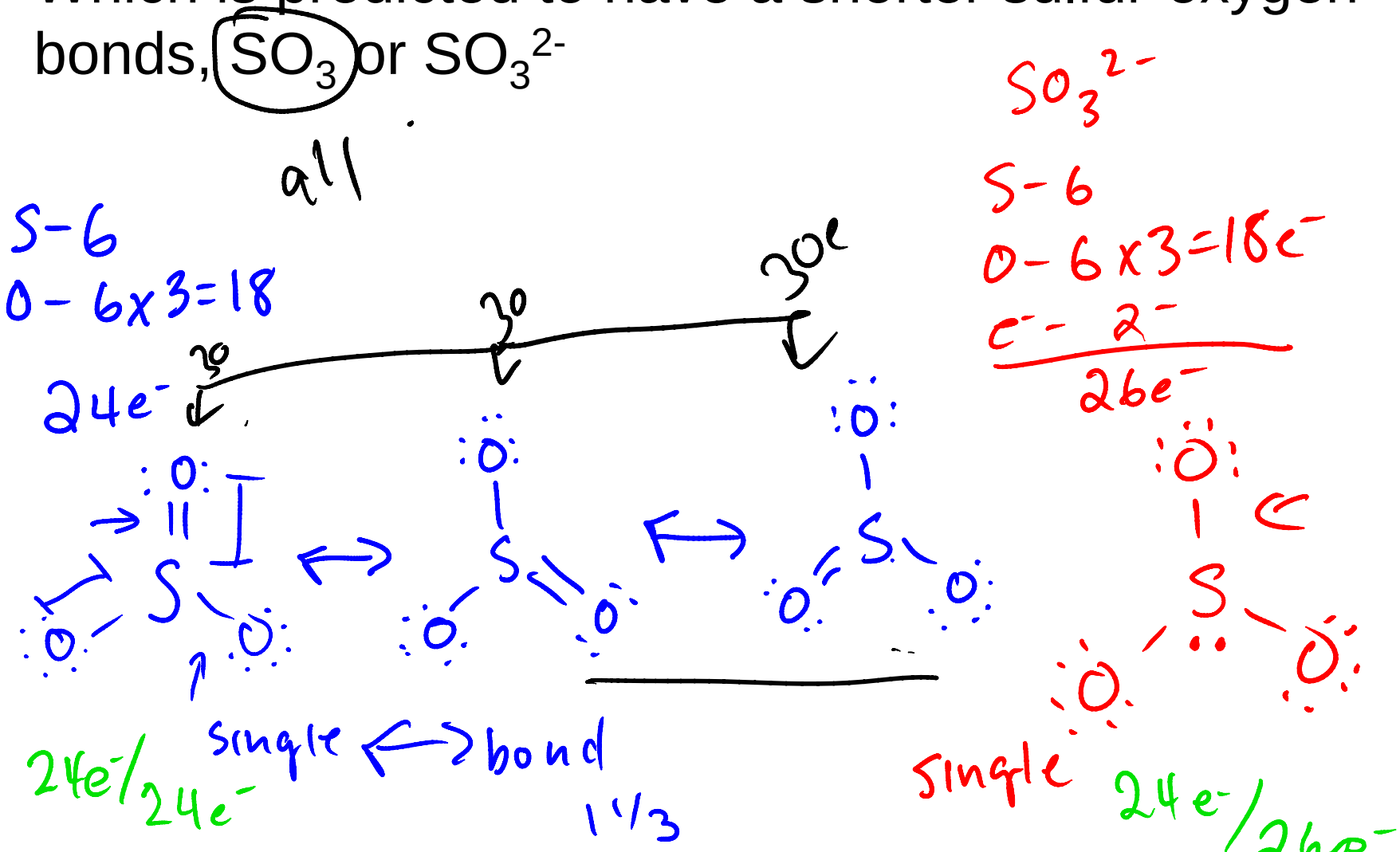
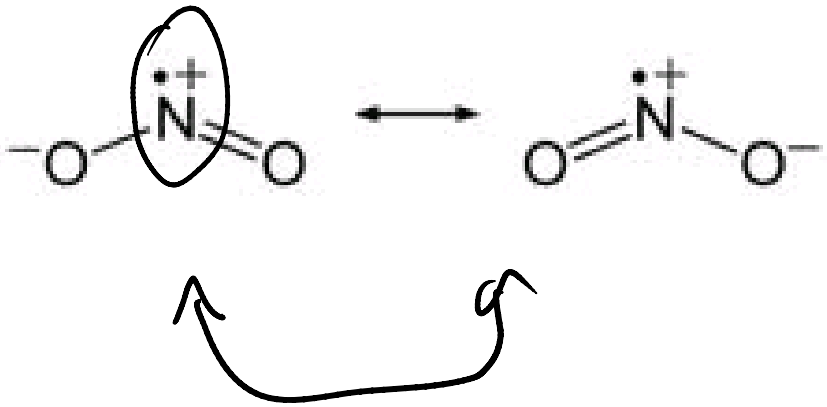
Resonance Structure

Which is predicted to have a shorter sulfur-oxygen bonds, SO_3 or SO_3^{2-}

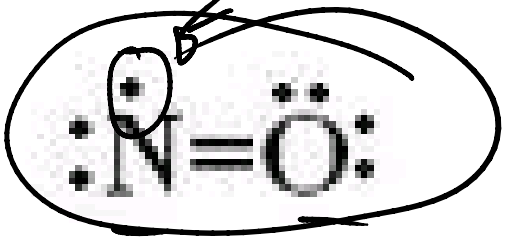


Odd Number of Electrons

Some stable molecules such as ClO_2, NO and NO_2 have and odd number of electrons.



free radical



N - 5

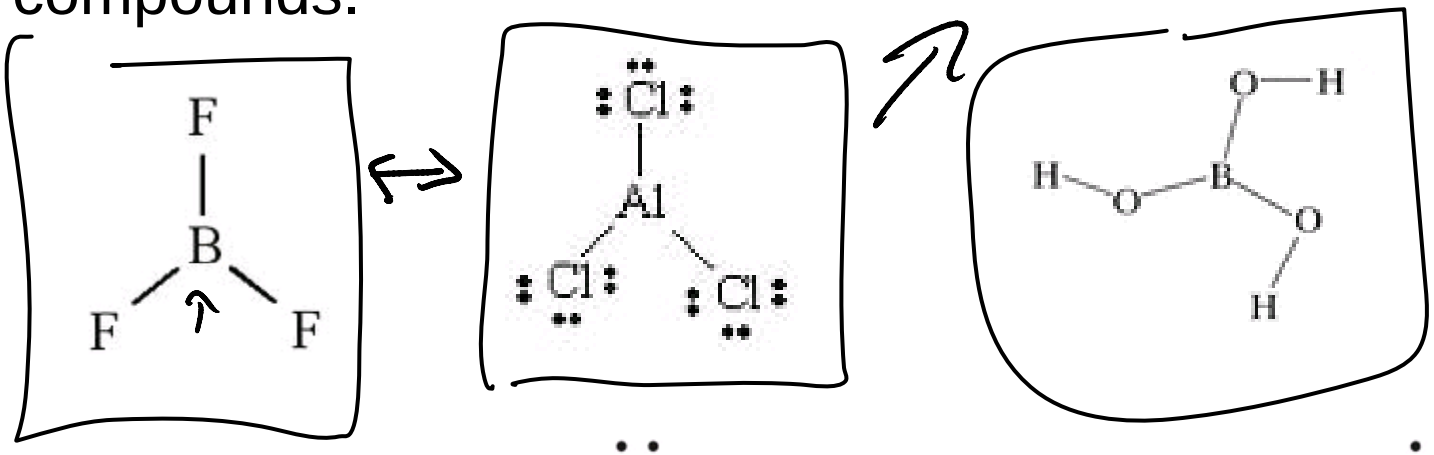
O - 6

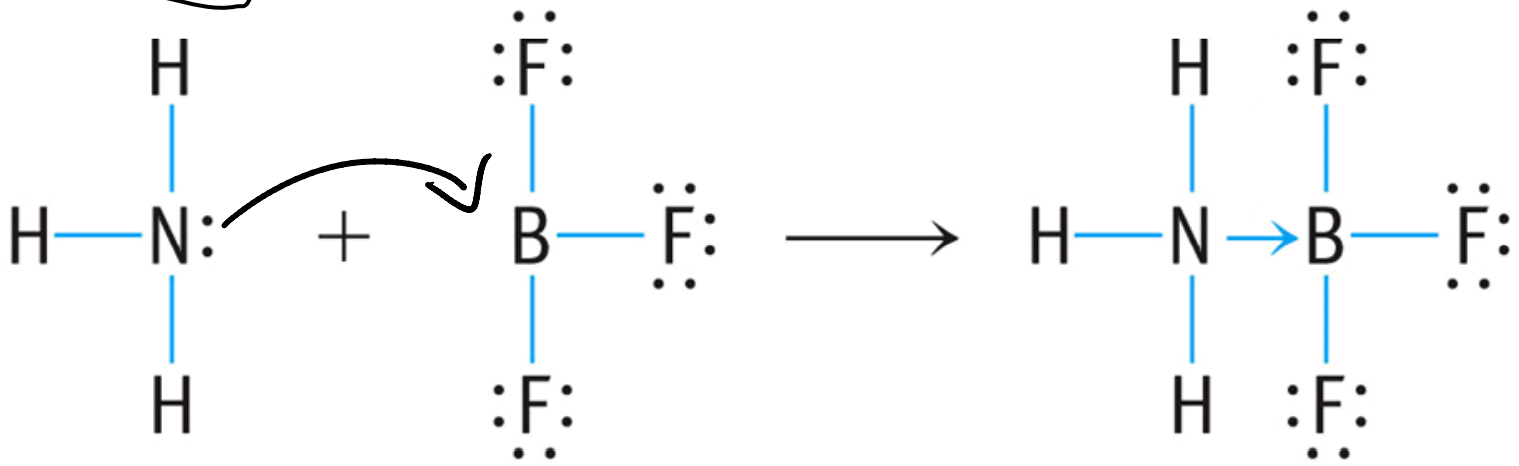
11

Less than an Octet

electron deficient

Rare case found in mainly boron, aluminum and beryllium compounds.





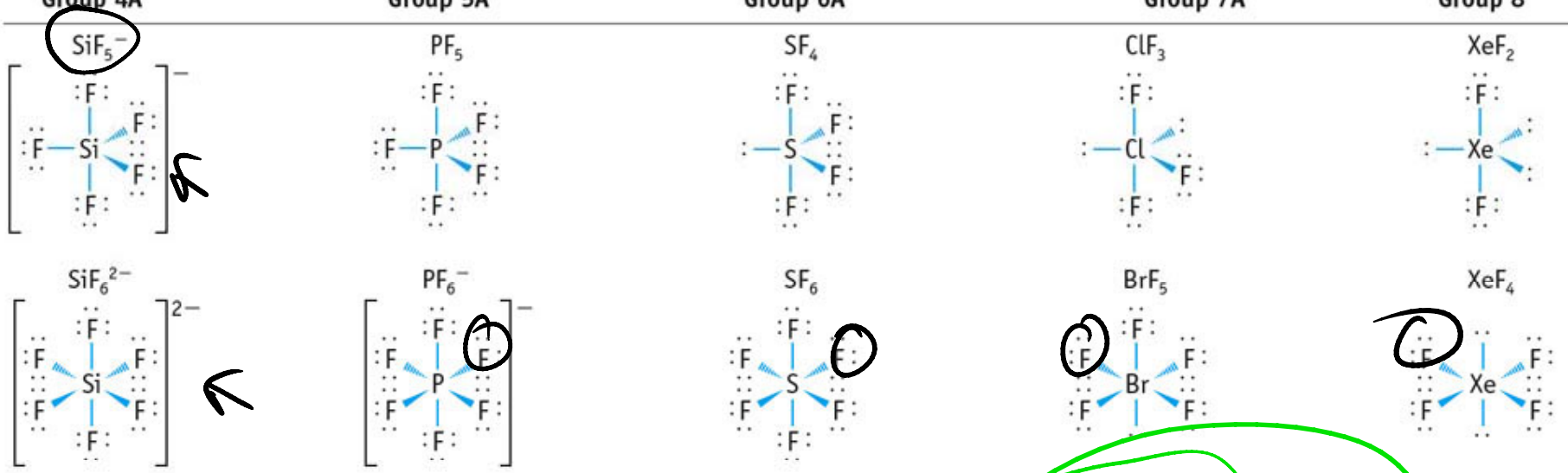
More than an Octet

hypervalence

Only happen with molecules where n =3 or greater

TABLE 8.6 Lewis Structures in Which the Central Atom Exceeds an Octet

Group 4A	Group 5A	Group 6A	Group 7A	Group 8
SiF_5^-	PF_5	SF_4	ClF_3	XeF_2
SiF_6^{2-}	PF_6^-	SF_6	BrF_5	XeF_4



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CNOF

d-orbital

Lewis

VSEPR (valence shell electron pair repulsion)

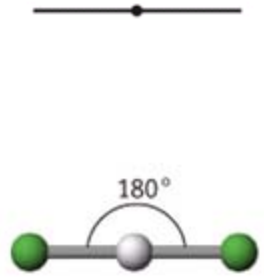
Molecular Geometry – is the arrangement of atoms in space.

Number of electron regions	Arrangement
2	Linear
3	Trigonal planar
4	Tetrahedral
5	Trigonal bipyramidal
6	Octahedral

- Basic Tenants
  - 1. Regions of high electron density - bp(s) + lp(s) - take up positions as far apart as possible.
  - 2. Molecular shape is determined by the resulting atomic positions
  - 3. lone pairs take up more space than bond pairs

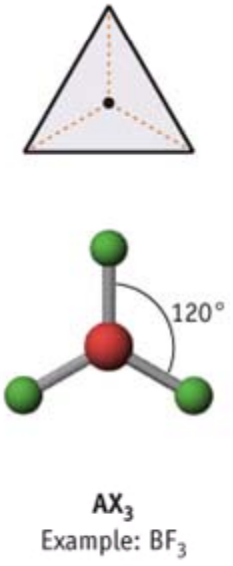
Shapes

- Linear



AX_2
Example: BeF_2

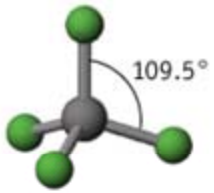
- Trigonal Planar



AX_3
Example: BF_3

Shapes

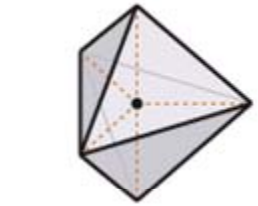
- Tetrahedral



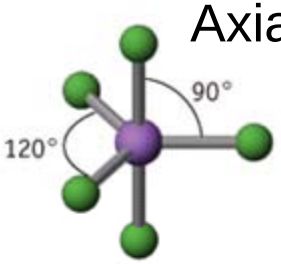
AX_4
Example: CF_4

Shapes

- Trigonal bipyramidal



Axial



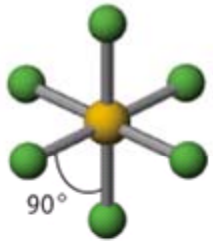
Equatorial

AX_5

Example: PF_5

Shapes

- Octahedral



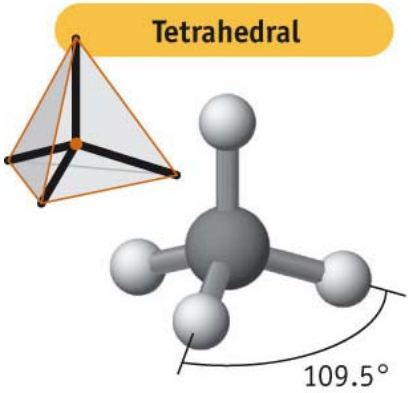
AX_6

Example: SF_6

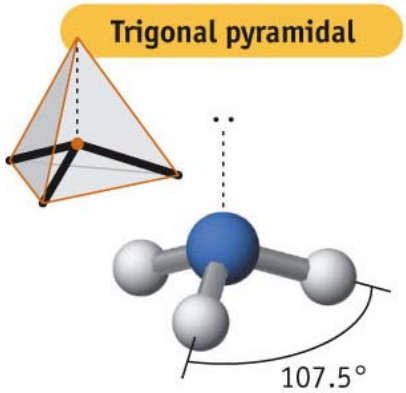
Lone Pair Geometry

- Lone pairs of electrons on the central atom occupy spatial positions.

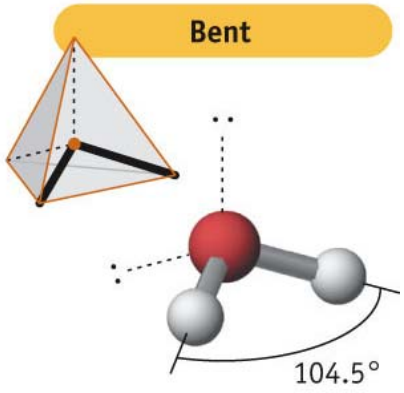
L.P.– L.P.> Lone Pair Bonding Pair > B.P. – B.P.



Methane, CH_4
4 bond pairs
no lone pairs

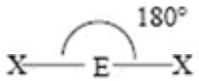
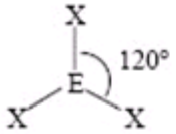
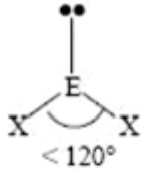
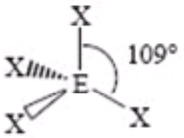
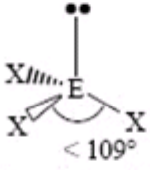
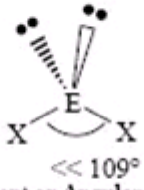
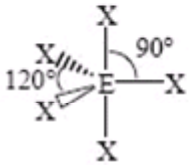
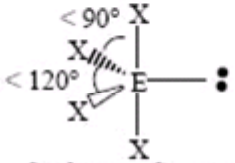
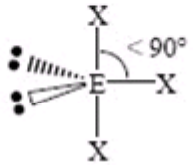
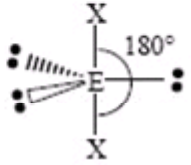
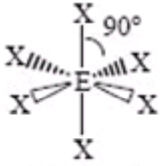


Ammonia, NH_3
3 bond pairs
1 lone pair



Water, H_2O
2 bond pairs
2 lone pairs

VSEPR

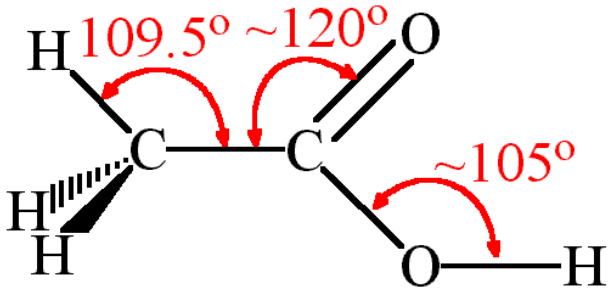
VSEPR Geometries					
Steric No.	Basic Geometry 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2	 Linear				
3	 Trigonal Planar	 Bent or Angular			
4	 Tetrahedral	 Trigonal Pyramid	 Bent or Angular		
5	 Trigonal Bipyramid	 Sawhorse or Seesaw	 T-shape	 Linear	
6	 Octahedral	 Square Pyramid	 Square Planar	 T-shape	 Linear

Molecular Geometry

1. Sketch the Lewis Structure.
2. Count the total number of electron pairs around the central atom (bonding and non-bonding) = steric number
3. Arrange electron pairs (bonding and non-bonding) on the central atom such that it minimizes electron pair replusion
4. Describe what shape you got.

** A double or triple bond is counted as one bonding pair when predicting geometry.

** Molecules with more than one “central atom” work the same way.

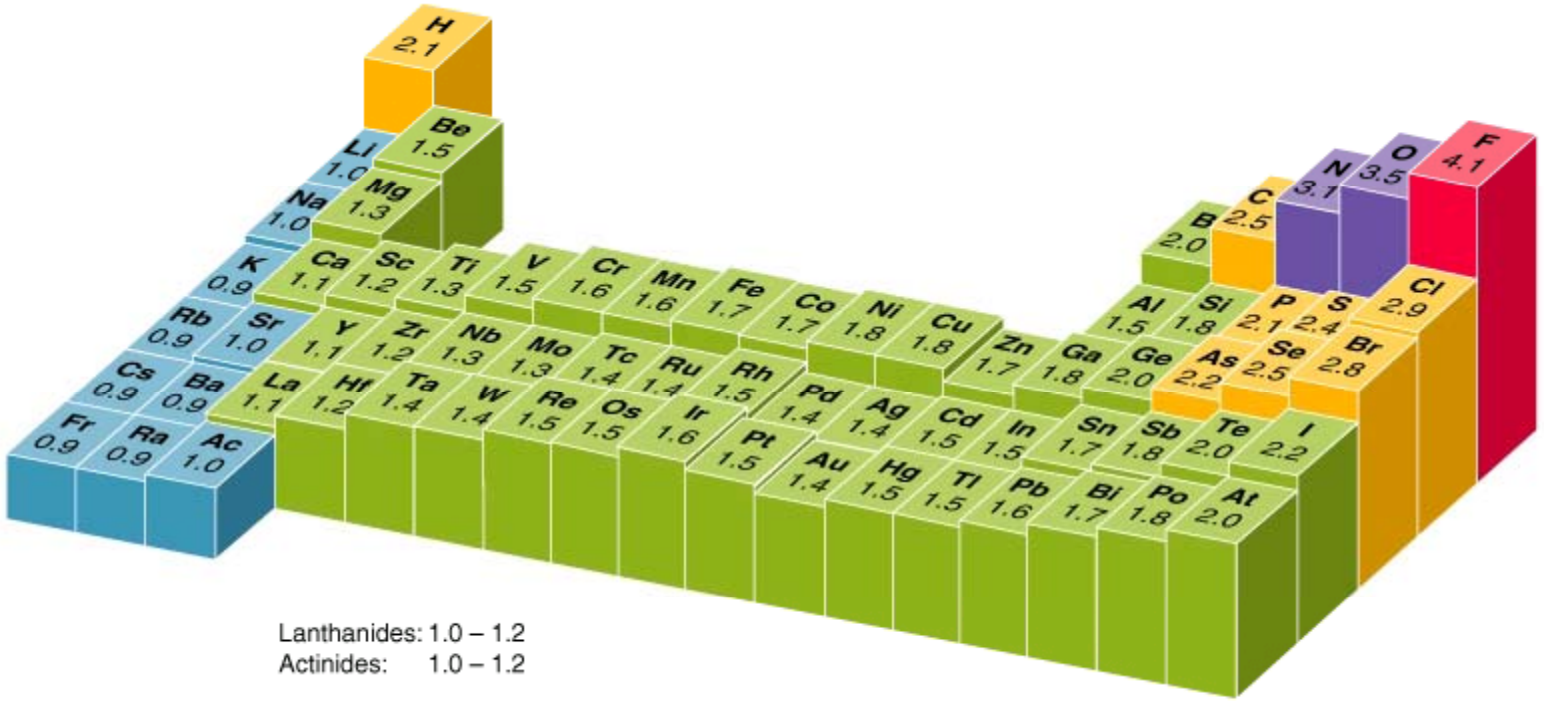


Let's Practice

Using VSEPR model, predict the molecular geometry of (a)SF_4 and IF_5

Electronegativity

- The power of an atom to attract electrons when it is part of a compound
- Mulliken - $\chi_m = 1/2\ (I + E_a)$



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