Chapter 10
Shapes of Molecules

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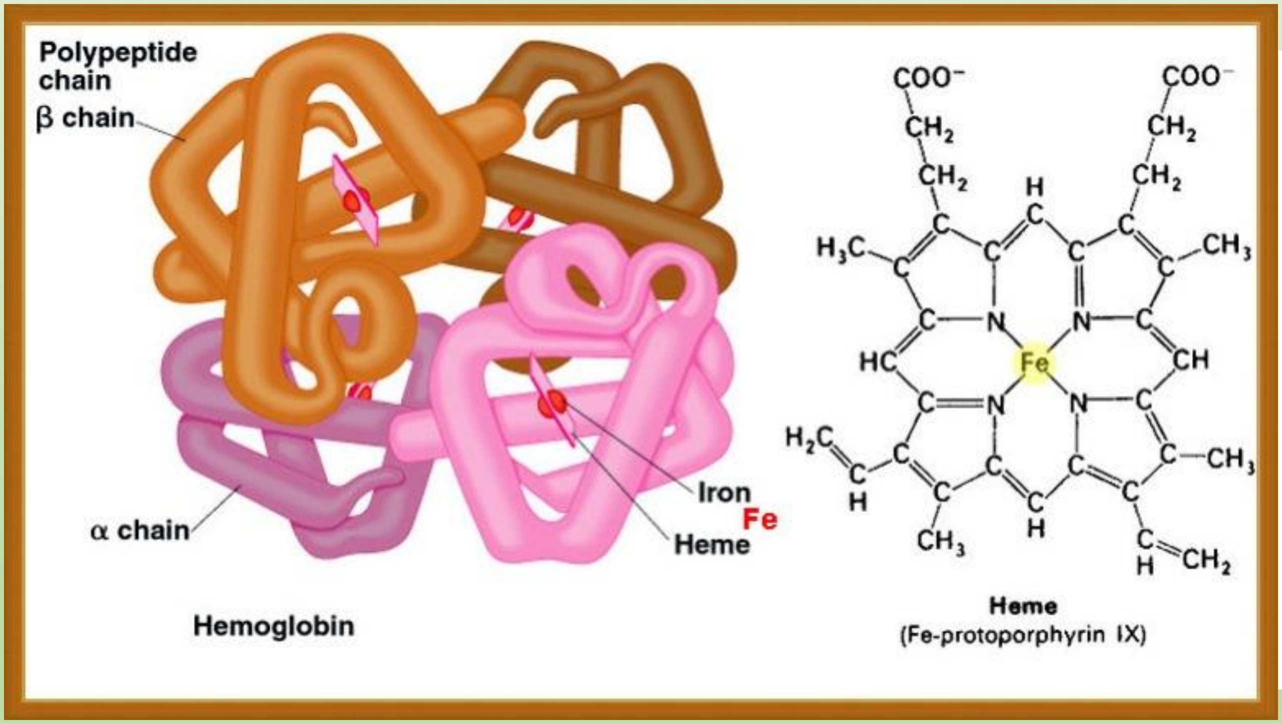
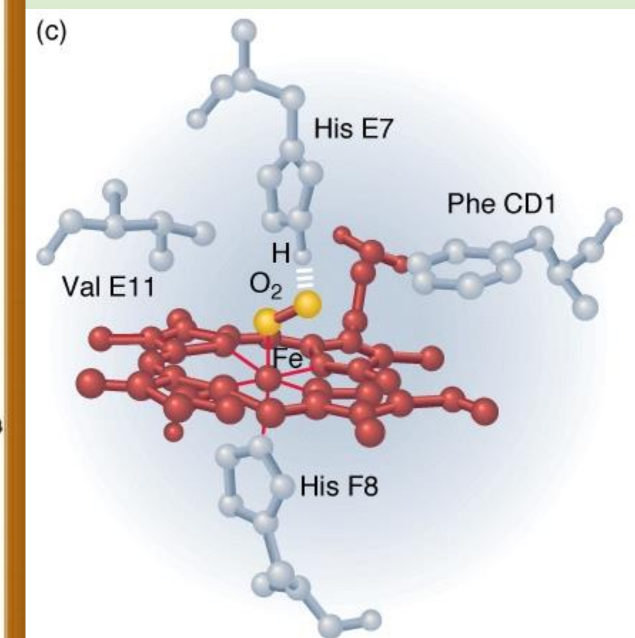
Shapes of Molecules - Importance

- All molecules have a 3D orientations; even the diatomic ones because atoms have a volume.
- In case of tri atomic or polyatomic molecules and ions these shapes can get very important.
- Physical properties of molecules can be predicted by the shape of molecule.
  - Why is H_2O liquid but CO_2 a gas at room temperature?
- Molecular interactions can be predicted by shape of molecule.
- A number of biological functions occur because of proper molecular interactions.
  - Hemoglobin and oxygen binding

Hemoglobin

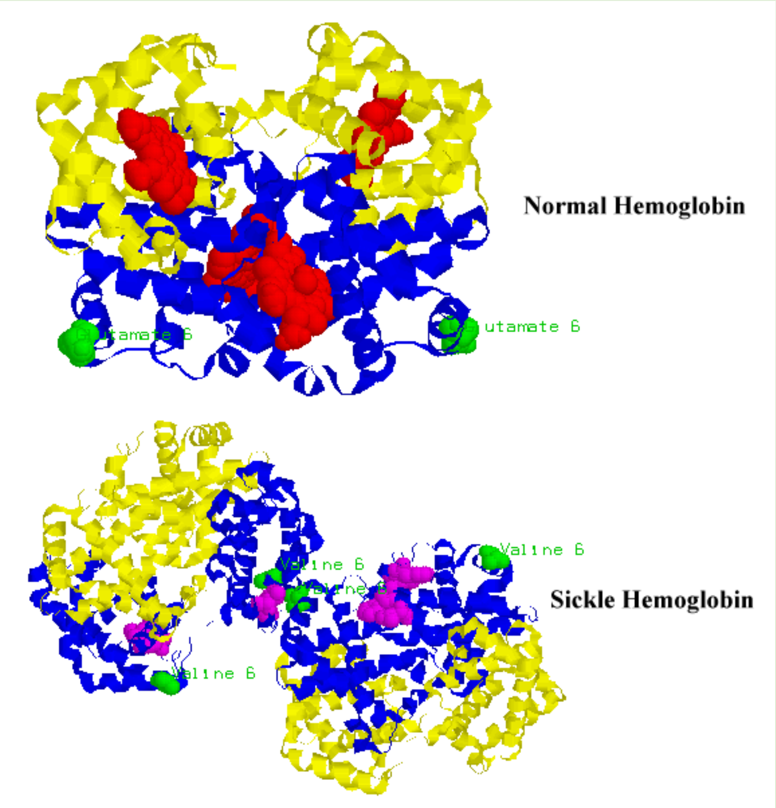
- 4 Protein subunits + 4 macromolecules (with metal) = hemoglobin
- Macromolecule is porphyrin with iron in the center for bonding with oxygen.



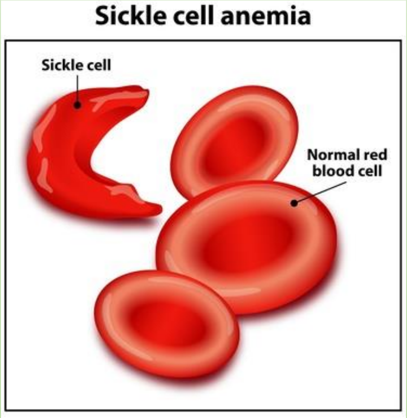


Hemoglobin - 2

Sickle cell anemia – inability of hemoglobin to bind to oxygen. Difference of one amino acid (glutamic acid is replaced by valine) changes the shape of the whole protein.

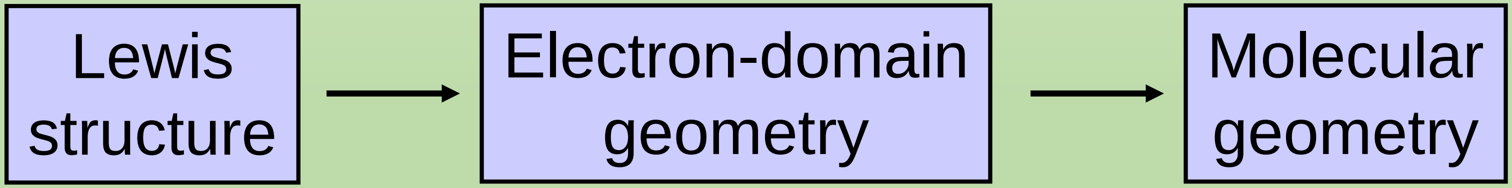


Note: The Sickle hemoglobin image is drawn at 50% of the size of the Normal hemoglobin



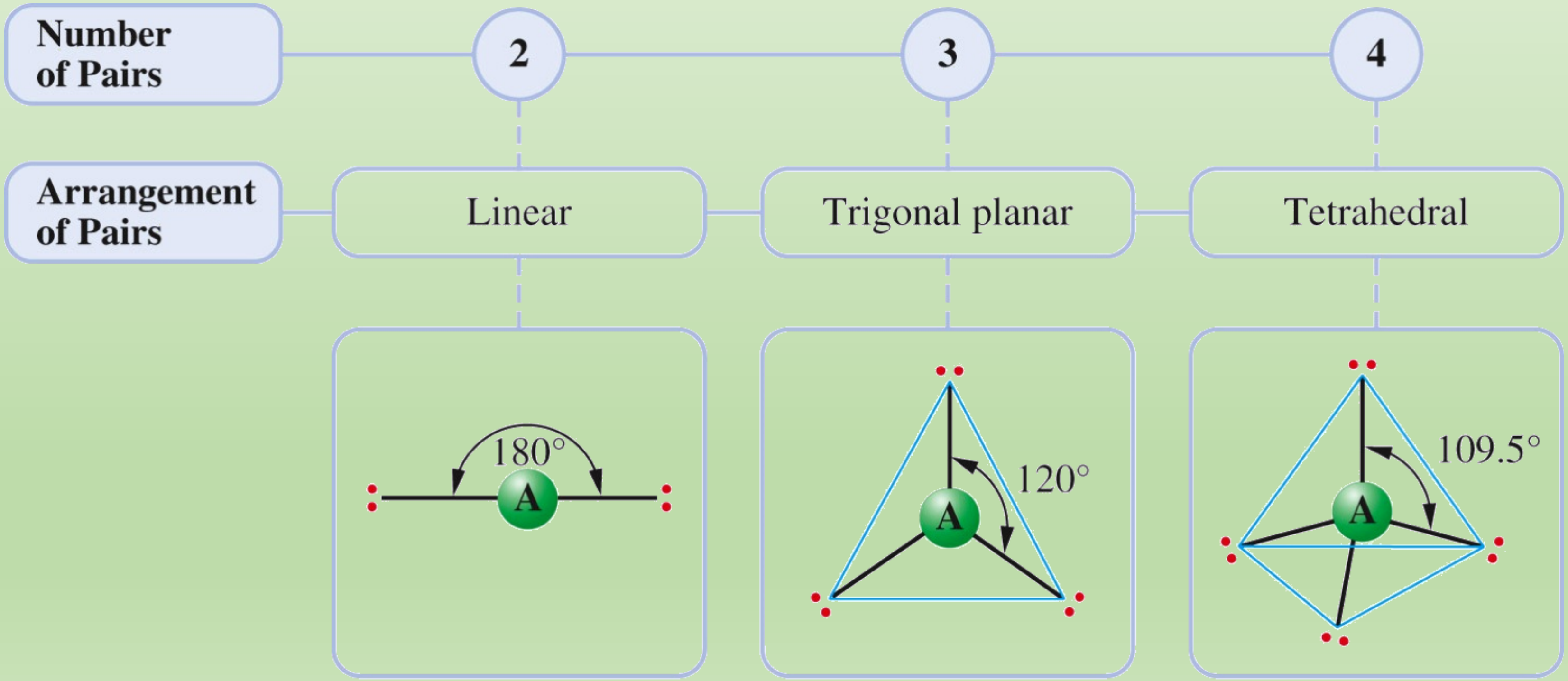
Molecular Geometry

- This is the three dimensional shape of a molecule.
- Geometry can be predicted by Lewis structures and VSEPR theory.
- VSEPR – Valence Shell Electron Pair Repulsion Theory. This theory indicates that electron pairs, bonding or non bonding on the central atom, move far away to minimize repulsion.
- Predict the geometry using the strategy below.



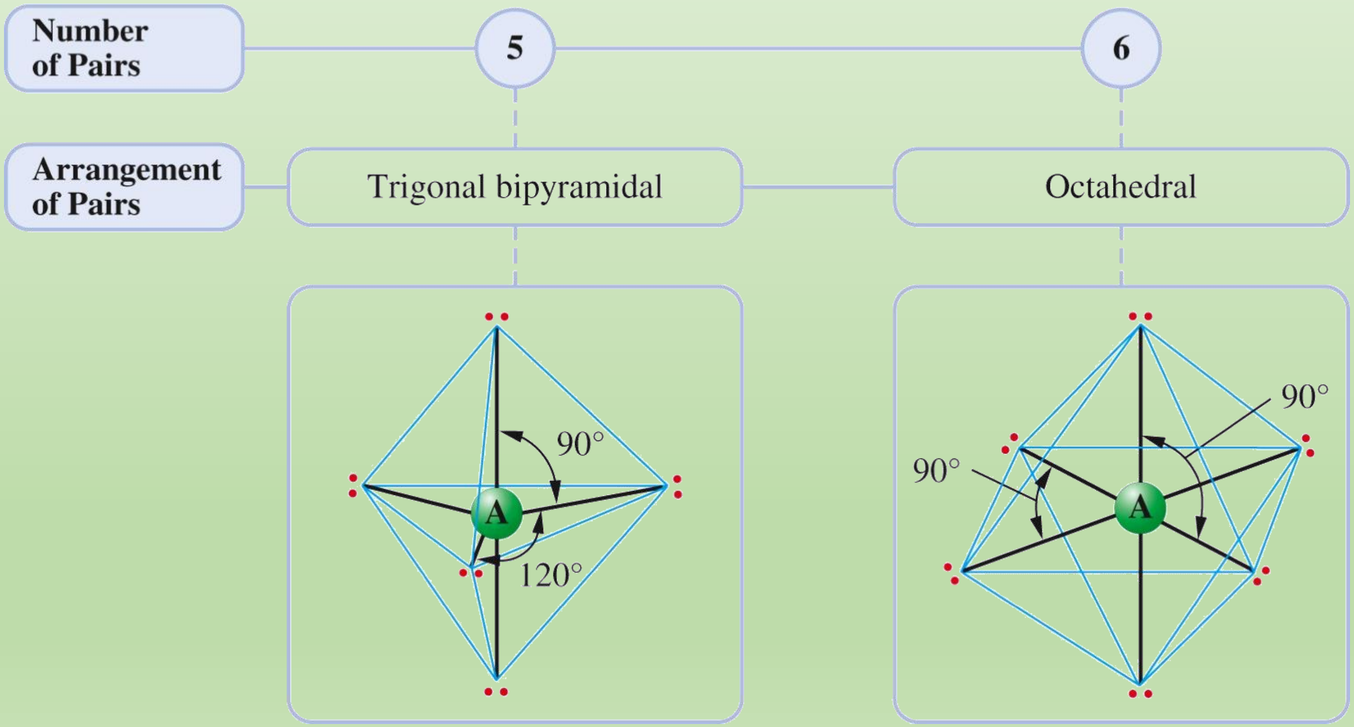
VSEPR- Shapes

- Two electron pairs are 180° apart (a linear arrangement).
- Three electron pairs are 120° apart in one plane (a trigonal planar arrangement).
- Four electron pairs are 109.5° apart in three dimensions (a tetrahedral arrangement).

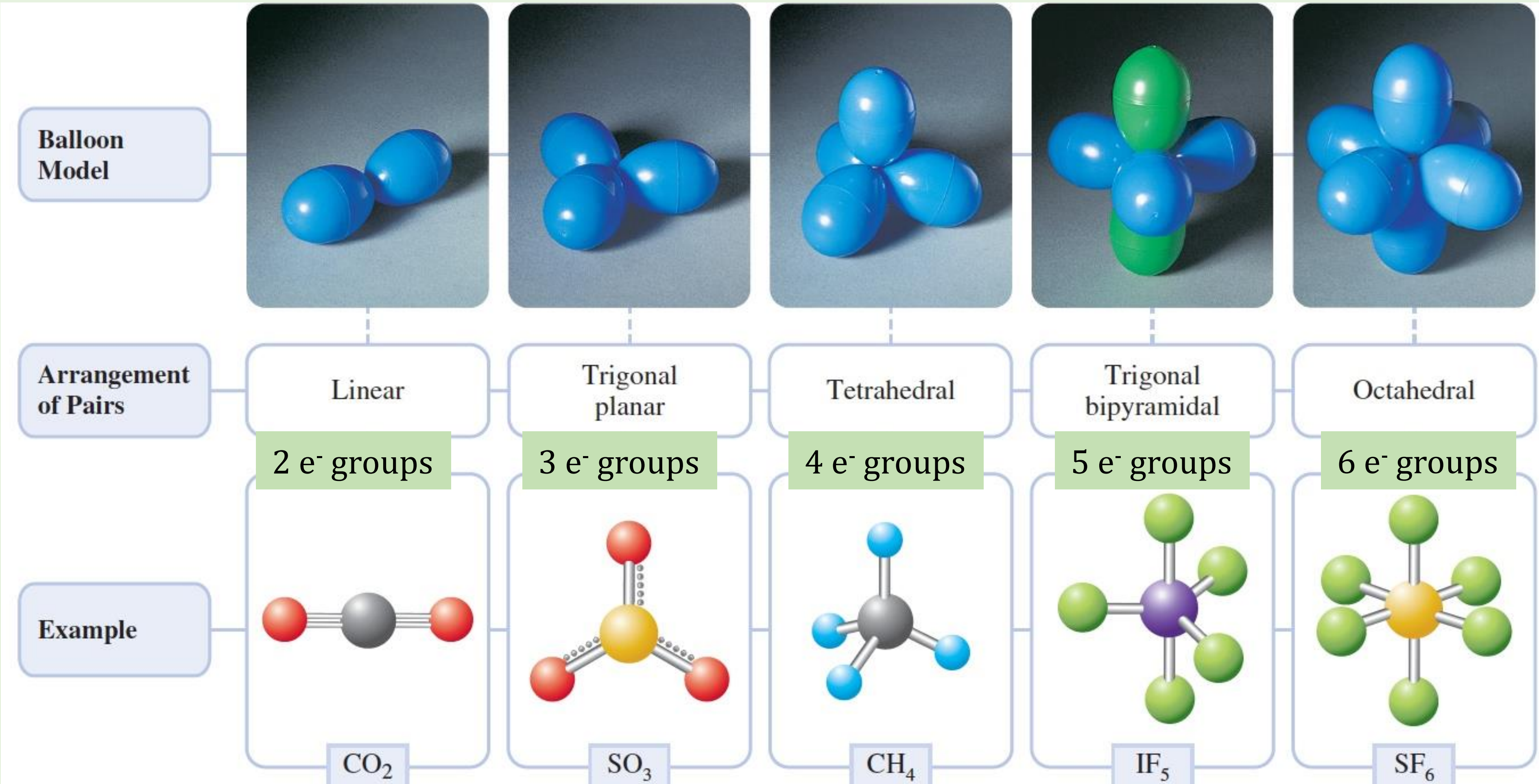


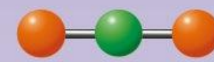
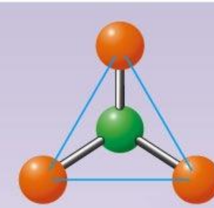
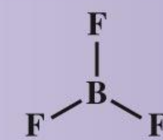
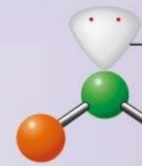
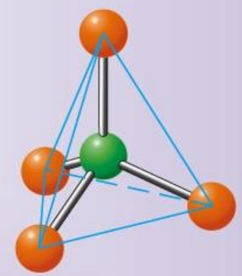
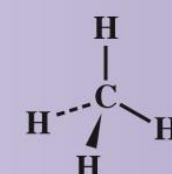
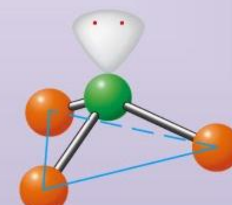
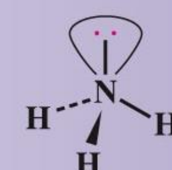
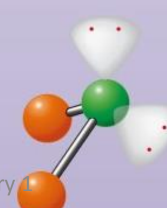
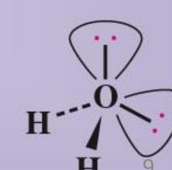
VSEPR – Shapes 2

- Five electron pairs are arranged with three pairs in a plane 120° apart and two pairs at 90°to the plane and 180° to each other (a trigonal bipyramidal arrangement).
- Six electron pairs are 90° apart (an octahedral arrangement).

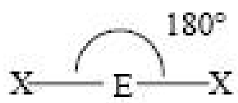
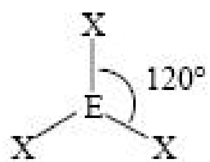
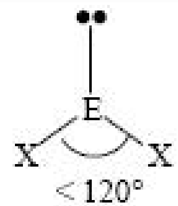
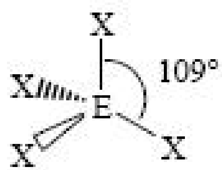
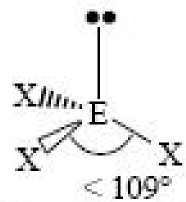
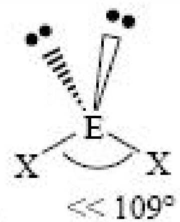
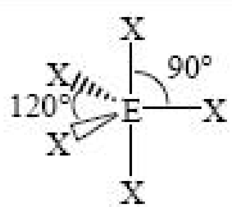
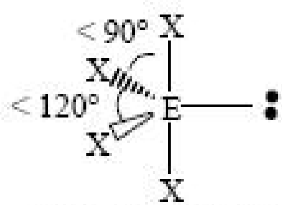
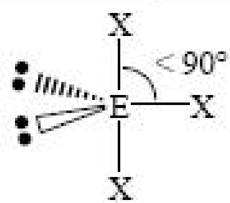
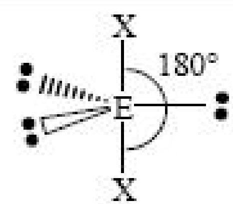
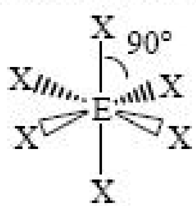
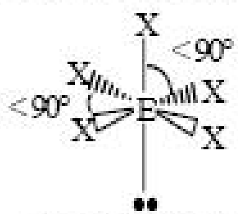
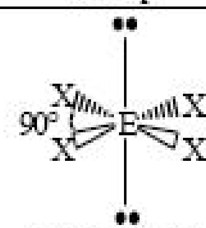
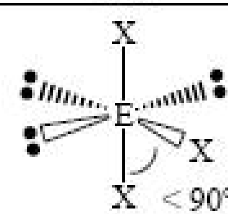
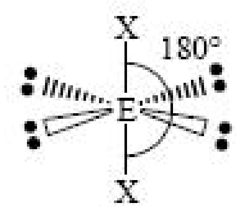


VSEPR – Shapes 3



Electron Pairs Total	Bonding	Lone	Arrangement of Pairs *Electron Geometry*	Molecular shape AXE	Molecular Geometry	Example	
2	2	0	Linear 180^o	Linear AX_2		BeF_2	F—Be—F
3	3	0	Trigonal planar 120^o	Trigonal planar AX_3		BF_3	
	2	1		Bent (or angular) AX_2E_1	 —Lone pair	SO_2	
4	4	0	Tetrahedral 109^o	Tetrahedral AX_4		CH_4	
	3	1		Trigonal pyramidal AX_3E_1		NH_3	
	2	2		Bent (or angular) AX_2E_2		H_2O	

Electron Groups	AXE formula	Bond Angle	E.g.	Electronic Geometry	Shape of Molecule
2	AX_2	180^{o}	$BeCl_2$	Linear	Linear
3	AX_3	120^{o}	BF_3	Trigonal planar	Trigonal planar
3	AX_2E	120^{o}	SO_2	Trigonal planar	Bent
4	AX_4	109.5^{o}	CH_4	Tetrahedral	Tetrahedral
4	AX_3E	109.5^{o}	NH_3	Tetrahedral	Trigonal Pyramidal
4	AX_2E_2	109.5^{o}	H_2O	Tetrahedral	Bent
5	AX_5	90^{o}, 120^{o}, 180^{o}	PCl_5	Trigonal bipyramidal	Trigonal Bipyramidal
5	AX_4E	90^{o}, 120^{o}, 180^{o}	SF_4	Trigonal bipyramidal	Seesaw
5	AX_3E_2	90^{o}, 180^{o}	CIF_4	Trigonal bipyramidal	T – shape
5	AX_2E_3	180^{o}	XeF_2	Trigonal bipyramidal	Linear
6	AX_6	90^{o}, 180^{o}	SF_6	Octahedral	Octahedral
6	AX_5E	90^{o}	BrF_5	Octahedral	Square Pyramidal
6	AX_4E_2	90^{o}	XeF_4	Octahedral	Square Planar
6	AX_3E_3	90^{o}, 180^{o}		Octahedral	T – Shape
6	AX_2E_4	180^{o}		Octahedral	Linear

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**

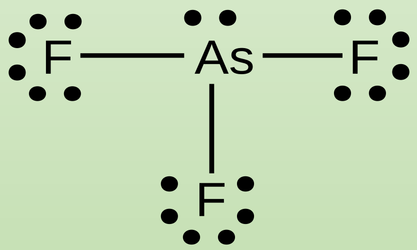
Solved Problem:

Use the VSEPR model to predict the geometries of the following molecules:

a. AsF_3

b. PH_4^+

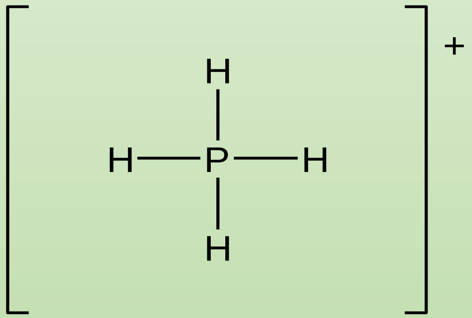
AsF_3 has 1(5) + 3(7) = 26 valence electrons; As is the central atom.



There are 4 pairs of electrons around As; three bonding and one lone pair.

The electronic geometry is tetrahedral. One of these regions is a lone pair, so the molecular geometry is trigonal pyramidal.

PH_4^+ has 1(5) + 4(1) – 1 = 8 valence electrons; P is the central atom.

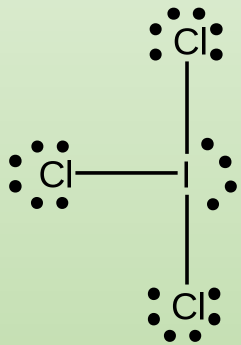


There are 4 pairs of electrons around P; all four bonding electron pairs.

The electronic geometry is tetrahedral. All regions are bonding, so the molecular geometry is tetrahedral.

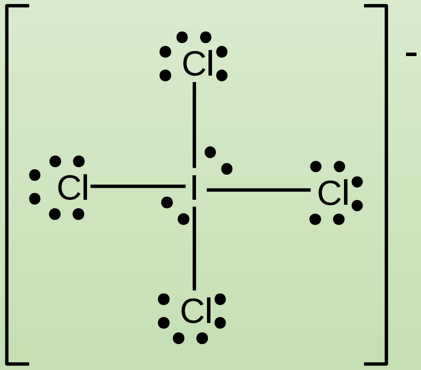
Solved Problem:
Use the VSEPR model to predict the geometries of the following molecules:
a. ICl_3
b. ICl_4^-

ICl_3 has 1(7) + 3(7) = 28 valence electrons. I is the central atom.



There are five regions: three bonding and two lone pairs.
The electronic geometry is trigonal bipyramidal.
The geometry is T-shaped.

ICl_4^- has 1(7) + 4(7) + 1 = 36 valence electrons. I is the central element



There are six regions around I: four bonding and two lone pairs.
The electronic geometry is octahedral.
The geometry is square planar.

Molecule with more than one Central Atom

For CH_3OH there are two central atoms so each will have its own geometry.

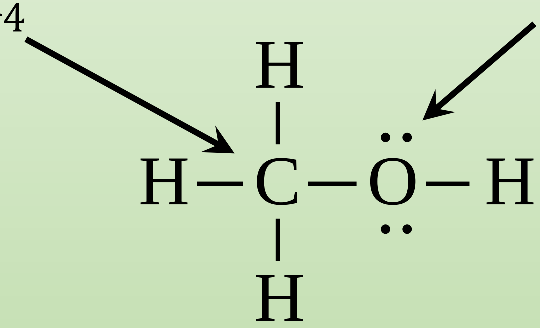
CH_3OH

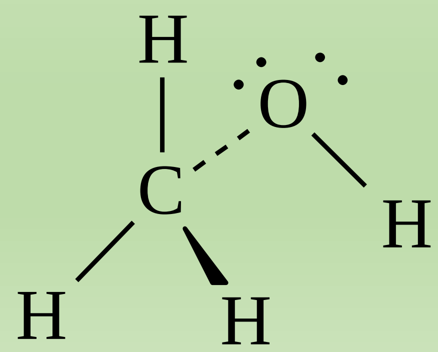
No lone pairs AX_4

tetrahedral

AX_4 2 lone pairs

bent





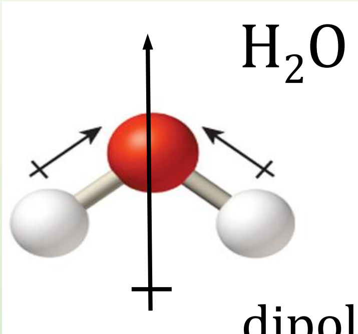
Dipole Moment and Polarity of Molecule

- Polarity is a degree of charge separation in a molecule
- For HCl, we can represent the charge separation using δ+ and δ- to indicate partial charges. Because Cl is more electronegative than H, it has the δ- charge, while H has the δ+ charge.

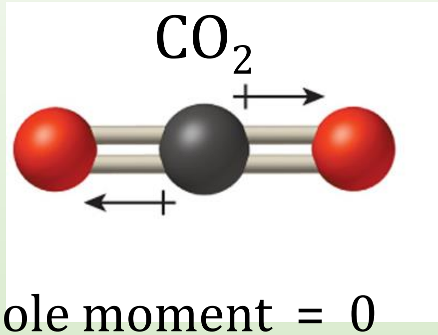
$$\overset{\delta+}{\mathrm{H}} \text{—} \overset{\delta-}{\mathrm{Cl}}$$

- Dipole moment a measure of how much a molecule can move in an electrical field. The movement occurs only if there is a charge separation.
- Polar molecules have dipole moment, while non polar molecules have zero dipole moment.
- To determine dipole moment:
    1. Draw the Lewis structure
    2. Determine the molecular shape of the molecule
    3. Determine the electronegativity from the periodic table
    4. See if the molecule is symmetrical as that will nullify the charge separation.
    5. Determine if the molecule is polar of not (yes – if molecule is asymmetric)

- Molecules with more than two atoms
  - Remember bond dipoles are additive since they are ***vectors***.

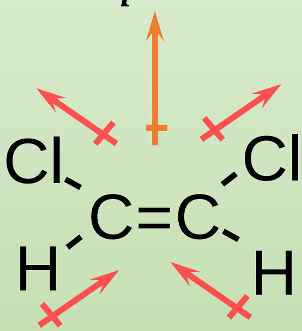


dipole moment > 0



dipole moment = 0

Example: Dichloroethene, $C_2H_2Cl_2$, exists as three isomers.

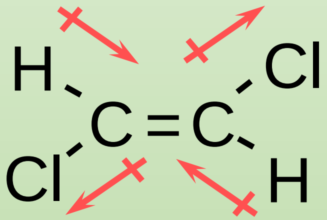


cis-1,2-dichloroethene

polar

μ = 1.90 D

bp = 60.3ºC

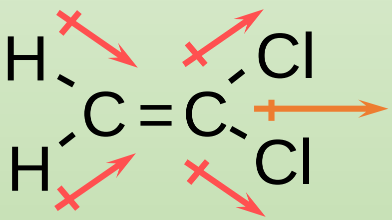


trans-1,2-dichloroethene

nonpolar

μ = 0 D

bp = 47.5ºC



1,1-dichloroethene

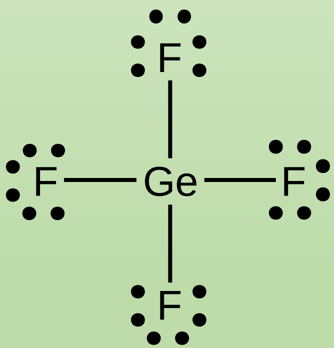
polar

μ = 1.34 D

bp = 31.7ºC

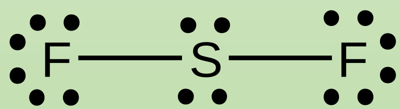
Solved Problem:
Which of the following molecules have dipole moment?
a. GeF_4 b. SF_2 c. AsF_3

GeF_4: 1(4) + 4(7) = 32 valence electrons.
Ge is the central atom.
8 electrons are bonding; 24 are nonbonding.
Tetrahedral molecular geometry. (AX_4)



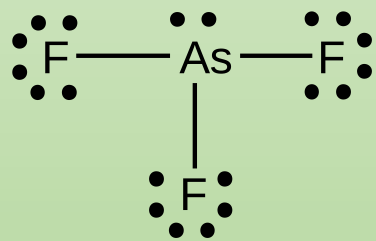
GeF_4 is nonpolar and has no dipole moment.

SF_2: 1(6) + 2(7) = 20 valence electrons.
S is the central atom.
4 electrons are bonding; 16 are nonbonding.
Bent molecular geometry. (AX_2E_2)



SF_2 is polar and has a dipole moment.

AsF_3: 1(5) + 3(7) = 26 valence electrons.
As is the central atom.
6 electrons are bonding; 20 are nonbonding.
Trigonal pyramidal molecular geometry. (AX_3E)



AsF_3 is polar and has a dipole moment.

Key Words/Concepts

- Molecular Geometry
- Shapes/VSEPR
- AXE formula
- Bonding and non bonding electrons
- Bond angles
- Electronegativity
- Bond polarity
- Polarity of molecule
- Dipole moment