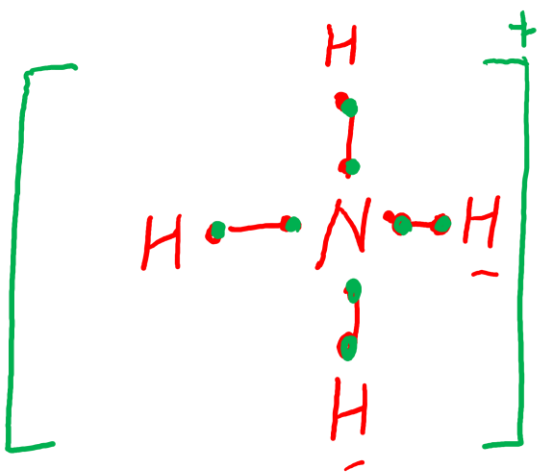
Assigning charges in polyatomic ions – Formal Charge Calculation

The **formal charge** of an atom in a molecule is the *hypothetical* charge the atom would have if we could redistribute the electrons in the bonds evenly between the atoms.

Assigning Formal Charge (FC)

1. Draw Lewis Structure
2. Determine neutral valence of each atom
3. Assign each atom half of bonding electrons + lone pairs
4. FC = valence electrons – lone pair electrons – (1/2) bonding electrons

ex. $[NH_4]^+$



$F.C_H = 1 - \left(\frac{2}{2}\right) = 0$

$F.C_N = 5 - \left(\frac{8}{2}\right) = +1$

Assigning Formal Charge

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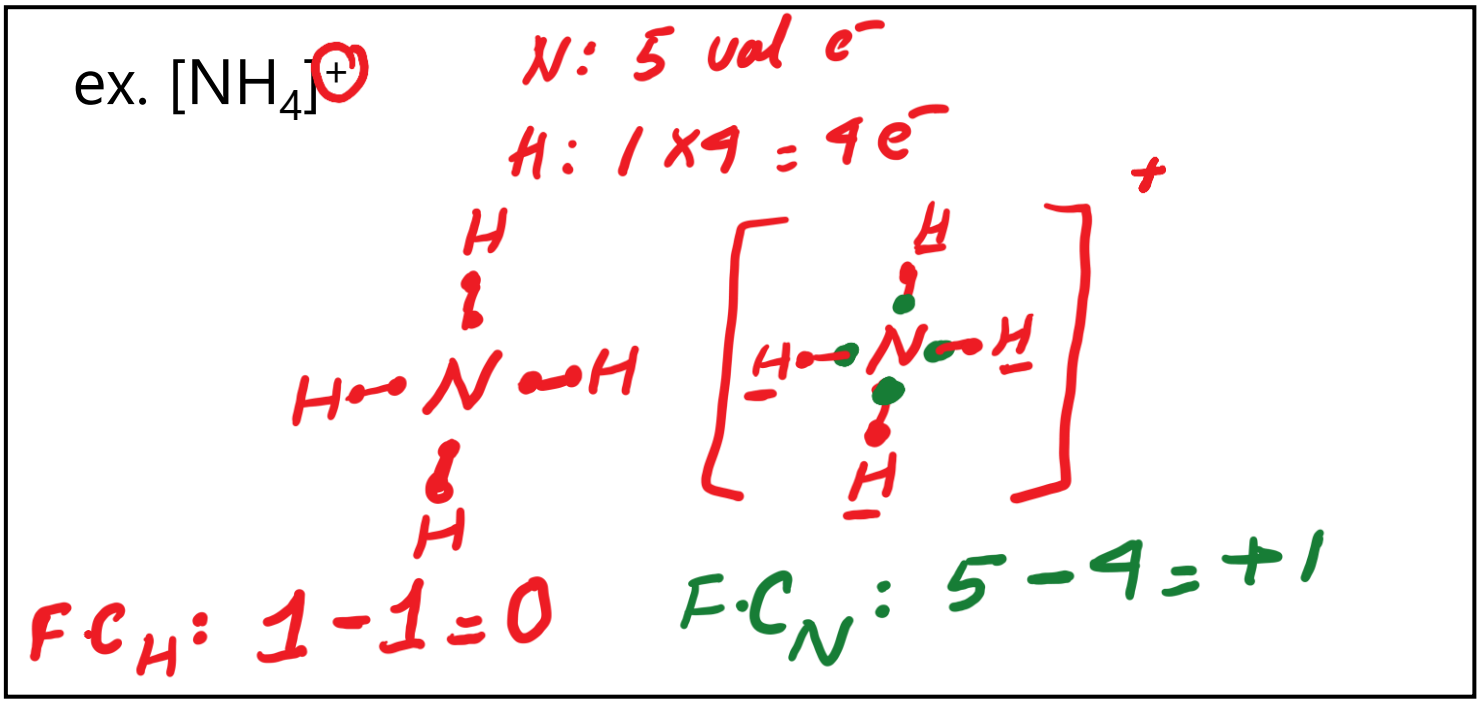


Determining the molecular structure

General Guidelines to determine the structure:

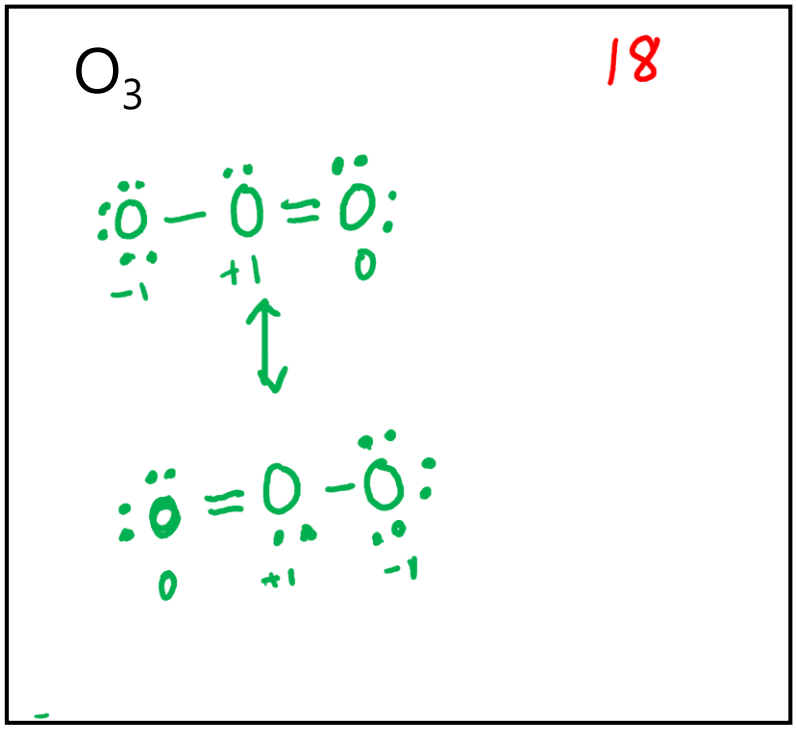
1. A molecular structure in which all formal charges are zero is preferable to one in which some formal charges are not zero.

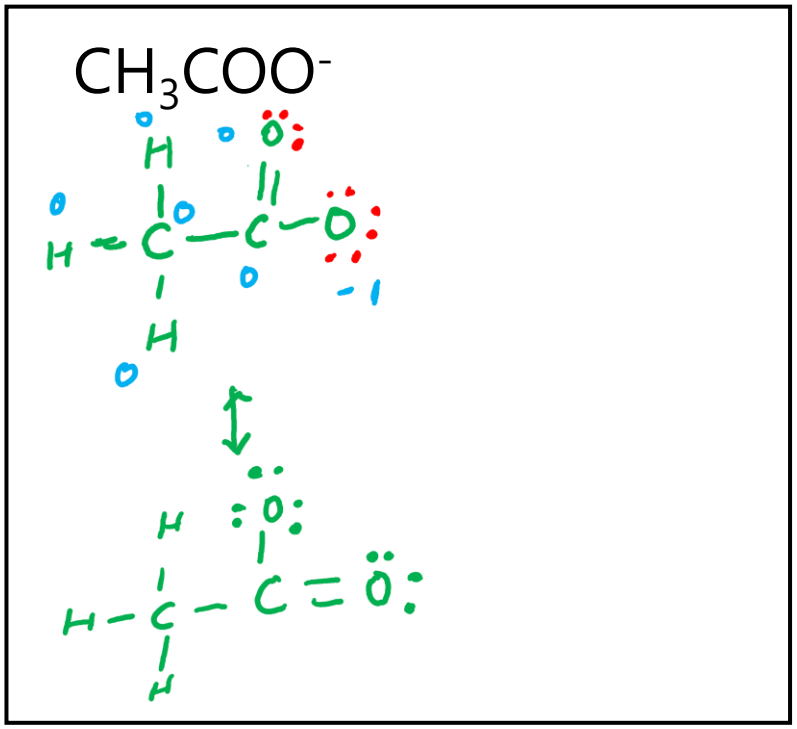
2. If the Lewis structure must have nonzero formal charges, the arrangement with the smallest nonzero formal charges is preferable.

3. Lewis structures are preferable when adjacent formal charges are zero or of the opposite sign.

4. When we must choose among several Lewis structures with similar distributions of formal charges, the structure with the negative formal charges on the more electronegative atoms is preferable.

Delocalized electrons in Lewis Structures: Resonance



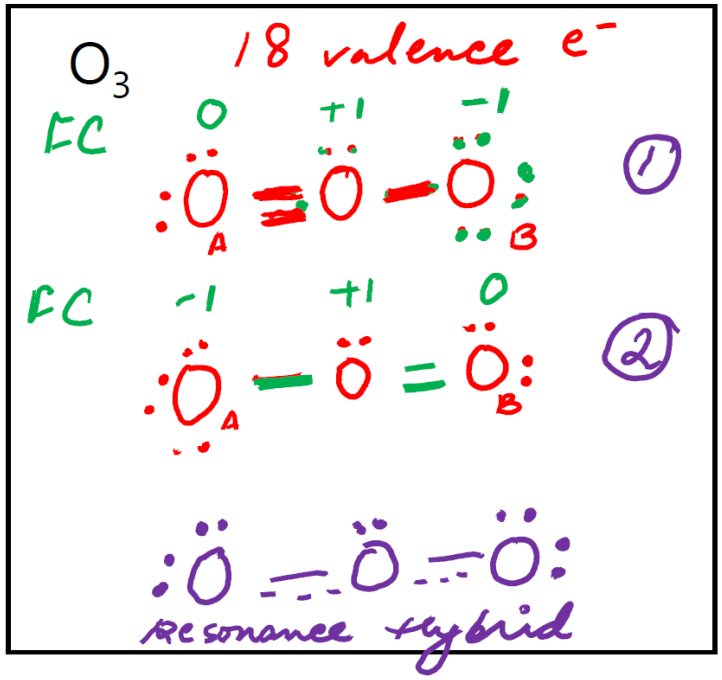


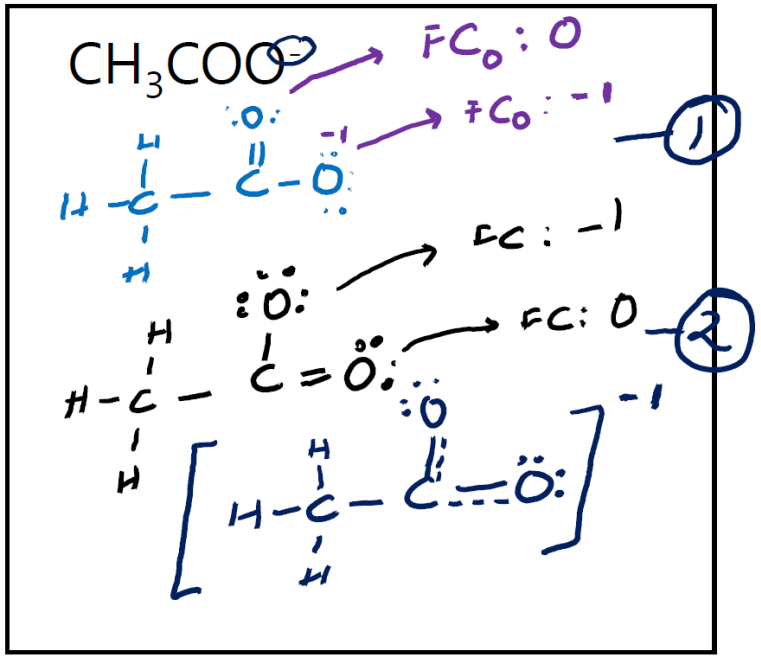
These multiple plausible structures for a molecule are called RESONANCE STRUCTURE

The electrons are ***delocalized*** over multiple bonds.

Movement of lone pairs/multiple bonds – Atoms DO NOT move

Delocalized electrons in Lewis Structures: Resonance





These multiple plausible structures for a molecule are called RESONANCE STRUCTURE

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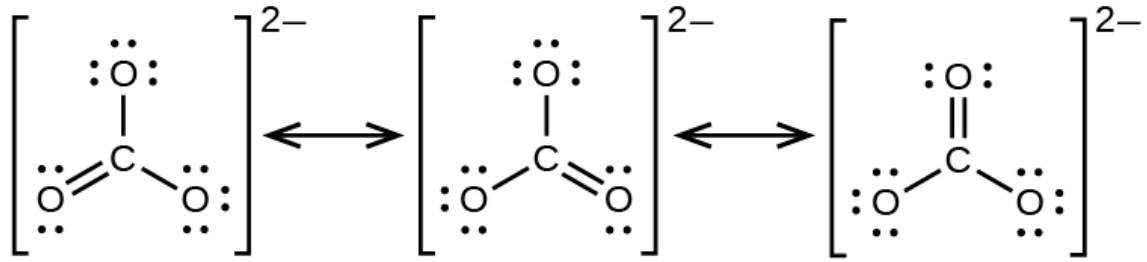
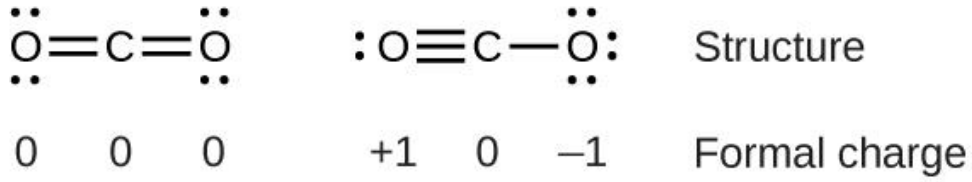
Determining the most contributing resonance structure



CO_3^{2-}

For carbonate ion shown above, all three resonance structures are equally contributing

But in some cases, different resonance structures have different formal charges on different atoms. CO_2 as an example:



Zero formal charge on all atoms is preferred - resonance structure with zero formal charge on more atoms preferred.

If the structure must have nonzero formal charges, the arrangement with the smallest nonzero formal charges is preferable

When we must choose among several structures with similar distributions of formal charges, the structure with the negative formal charges on the more electronegative atoms is preferable.

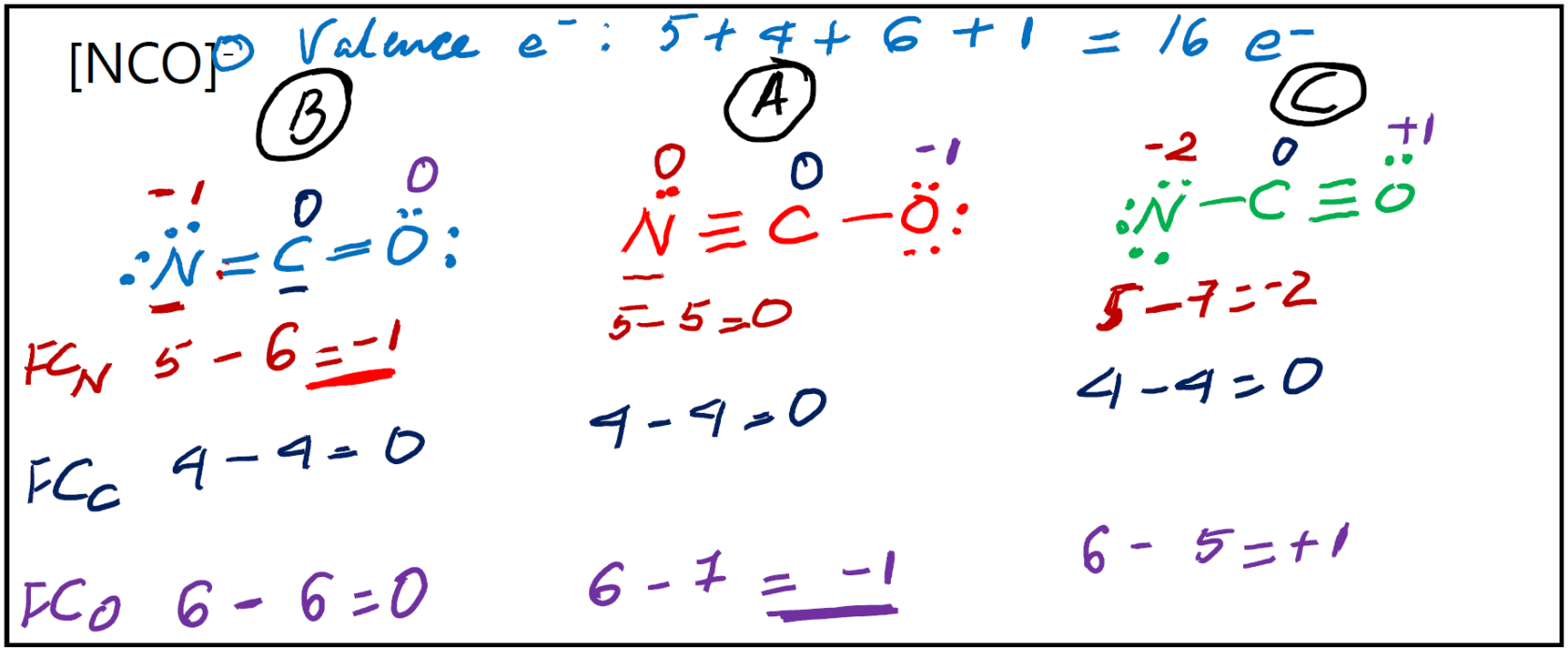
Delocalized electrons in Lewis Structures: Resonance

Draw three possible resonance structures for the following:

$[NCO]^-$

1. Resonance structures only exist on paper
2. Move electrons ONLY – not atoms
3. ALL structures must be **valid** Lewis structures
4. The ACTUAL structure is a **"hybrid"** of all resonance structures

Delocalized electrons in Lewis Structures: Resonance



All resonance structures must obey octet rule

O more electronegative than N

Picking best contributing/representative resonance structure:

- If the formal charges are the same, then –ve charge on most electronegative atom and +ve on least electronegative atom

A in $[NCO]^-$ has -1 on the most electronegative atom – this is the most contributing Lewis Structure

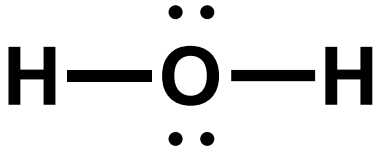
So far we have learned about the bonding between atoms – for the final part we will learn about how these electrons in a bond/molecule determine the overall shape of the molecule and how it affects the properties

Shapes of Molecules **(Concept Videos 14 and 15)**

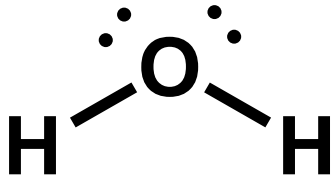
What will you be learning? Learning Objectives:

- Describe the six basic electronic geometries (base-shapes).
- Predict base-shape and molecular geometry for a molecule/complex ion using VSEPR theory.
- Describe how molecular shape effects overall polarity.

Lewis structures show bonds but not the geometry or shape of the molecule

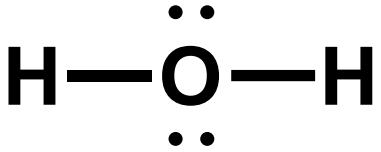


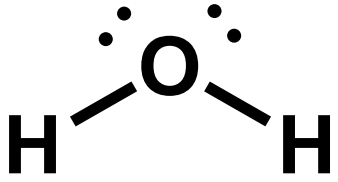
vs.



Molecular Geometry

Three-dimensional arrangement of the molecule depicting the bond length and bond angles



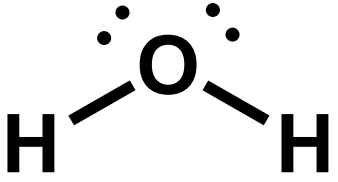


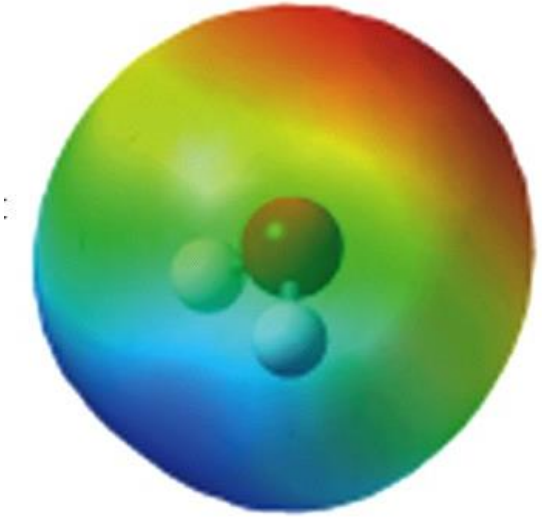
Lewis structures show bonds but not the geometry or shape of the molecule

Molecular Geometry

Why should we care about molecular geometry?

1. **Molecular Polarity**
2. Physical Properties (Intermolecular Forces)
3. Binding
4. Reactivity





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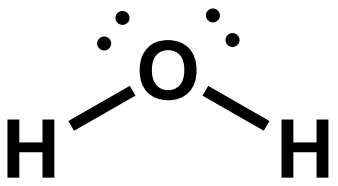

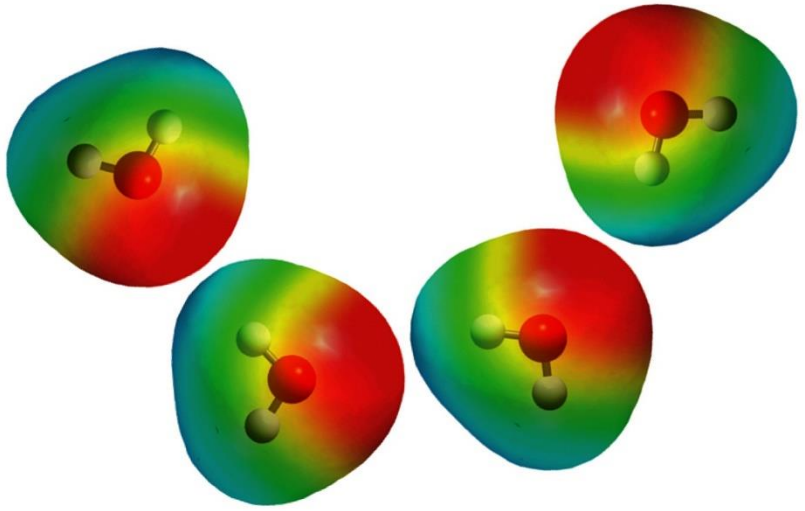

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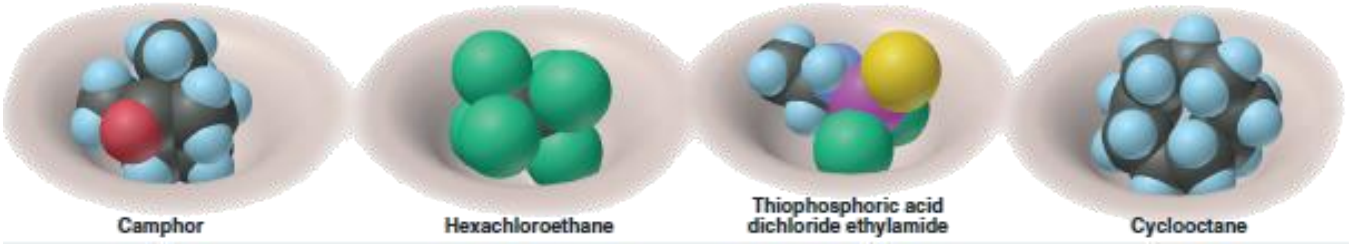
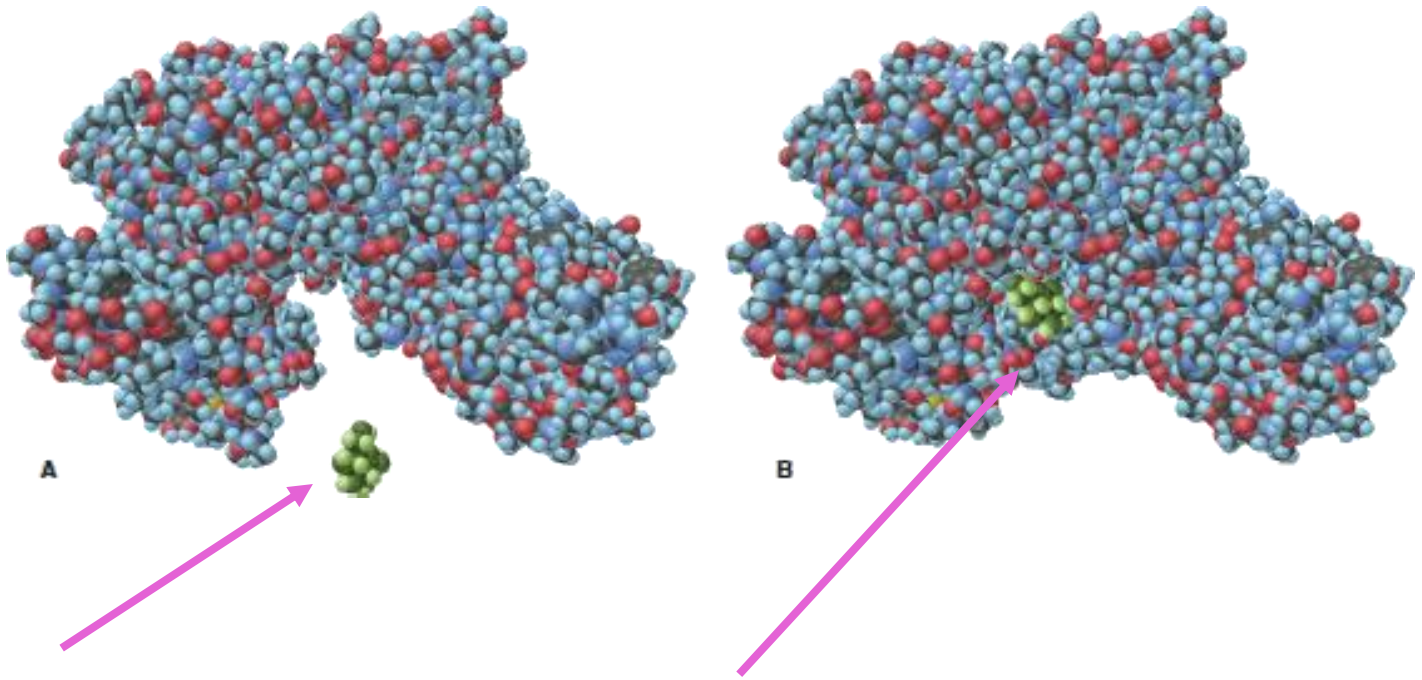


Sense of smell depends upon the shape of molecules (among many other things)

Molecular Geometry

Why should we care about molecular geometry?

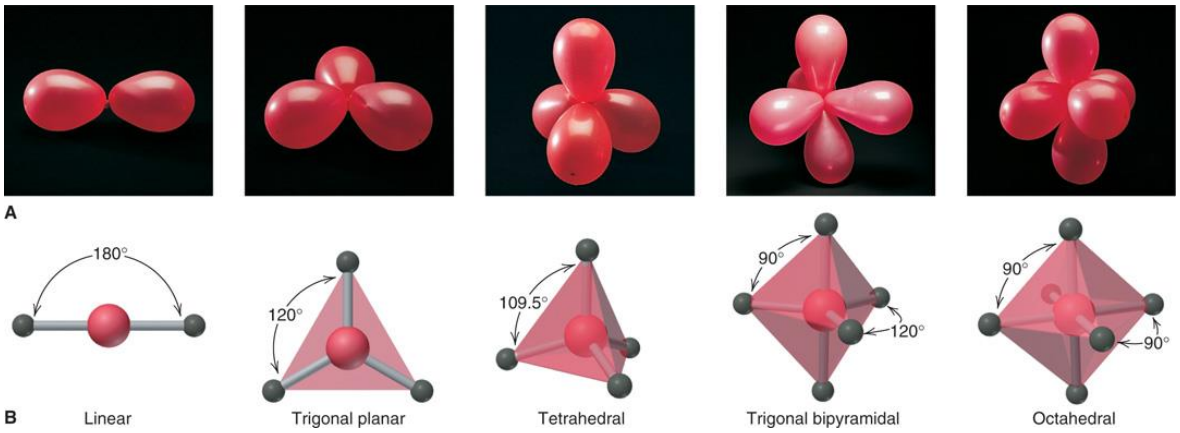
1. Molecular Polarity
2. Physical Properties (Intermolecular Forces)
3. Binding
4. **Reactivity**

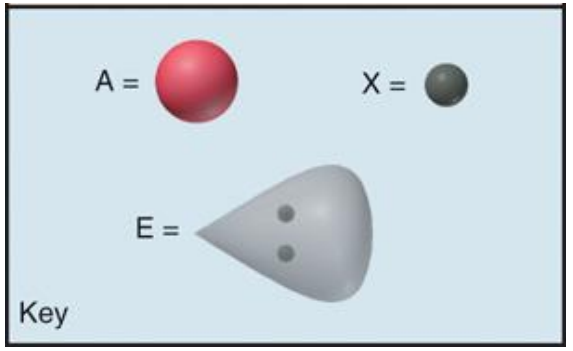


Determining Molecular Geometry Using VSEPR

VSEPR: *V*alence *S*hell *E*lectron *P*air *R*epulsion Theory

- Maximize space between valence *ELECTRON GROUPS* around an atom.
- One *ELECTRON GROUP* can be a:
    a) Lone pair
    b) Single bond
    c) Multiple bond
    d) Single unpaired electron





Molecule AX_2

Linear Geometry (AX_2)

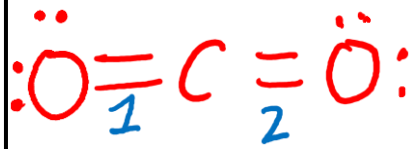
2 electron groups : 2 bonding groups (no lone pairs)

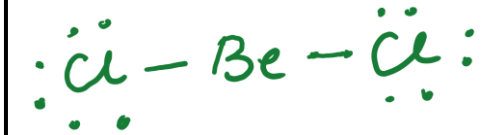
Bond Angle (XAX): 180˚

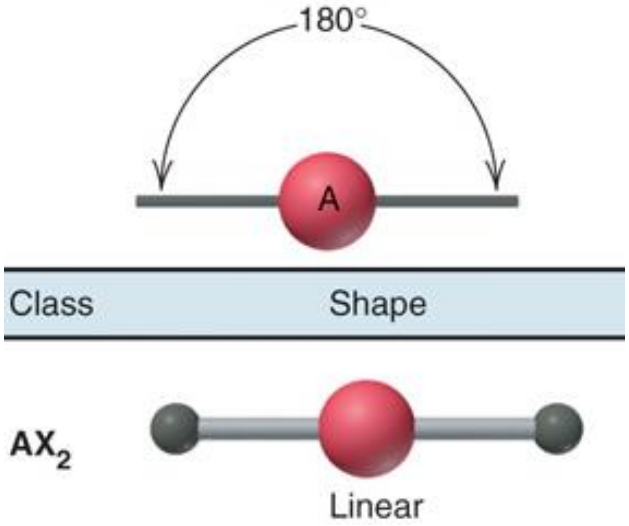
ex. CO_2, $BeCl_2$

EG = 2

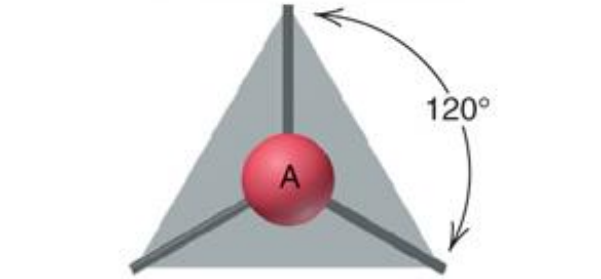
Bonding G = 2



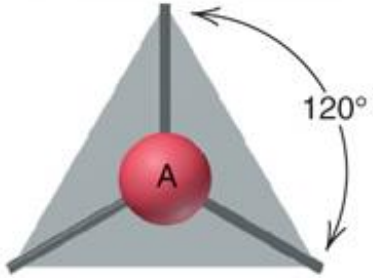




Three electron groups



Class	Shape
AX_3	Trigonal planar



Class	Shape
AX_2E	Bent (V shaped)

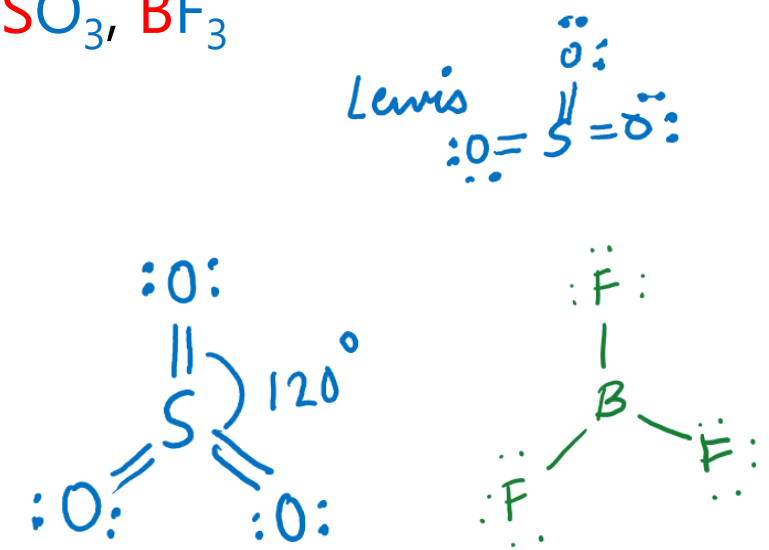
Molecule AX_3 (3 total electron groups)

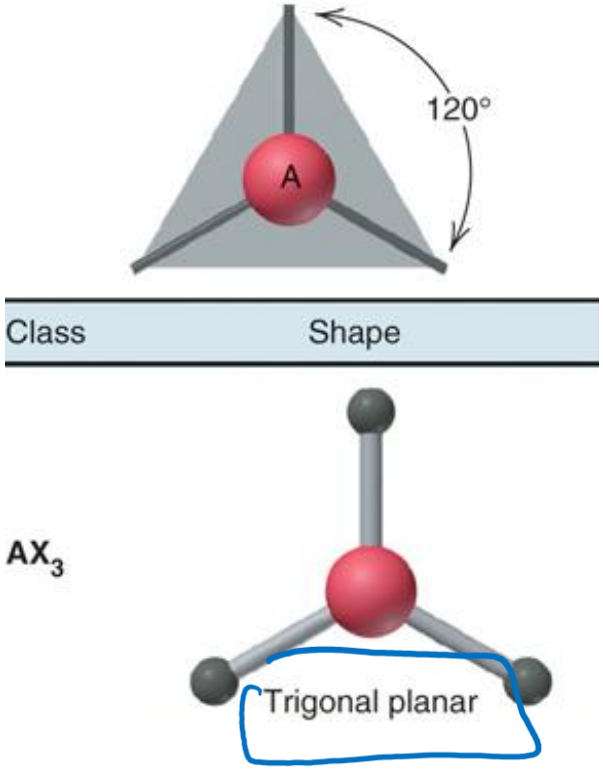
Trigonal Planar (AX_3)

3 electron groups : 3 bonding groups (no lone pairs)

Bond Angle (XAX): 120˚

ex. SO_3, BF_3





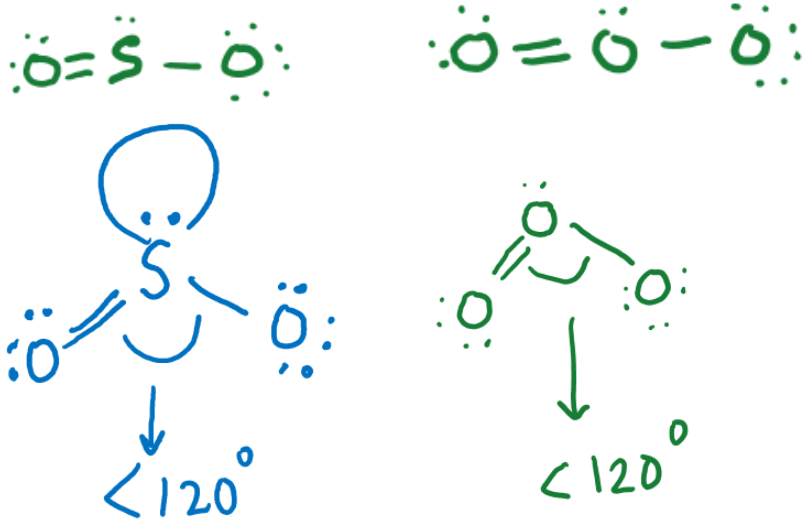
Molecule AX_2E (3 total electron groups)

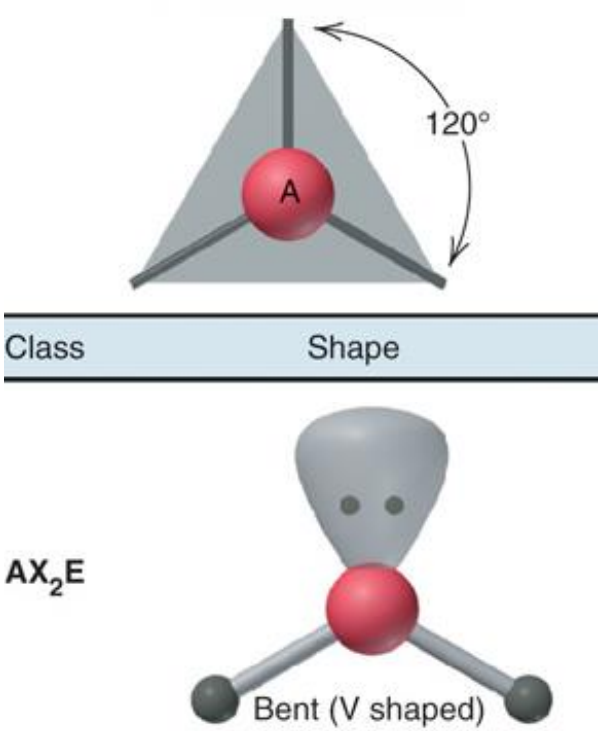
Bent Geometry (AX_2E)

3 electron groups : 2 bonding groups + 1 lone pair

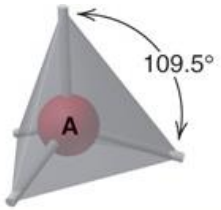
Bond Angle (XAX): ??

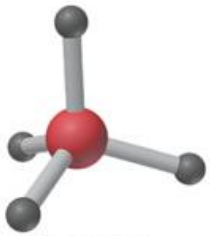
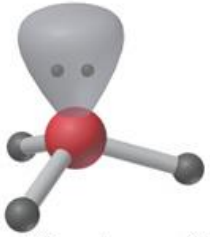
ex. SO_2, O_3





Four electron groups



Class	Shape
AX_4	 Tetrahedral
Examples: CH_4, $SiCl_4$, SO_4^{2-}, ClO_4^-	
AX_3E	 Trigonal pyramidal
Examples: NH_3, PF_3, ClO_3^-, H_3O^+	
AX_2E_2	

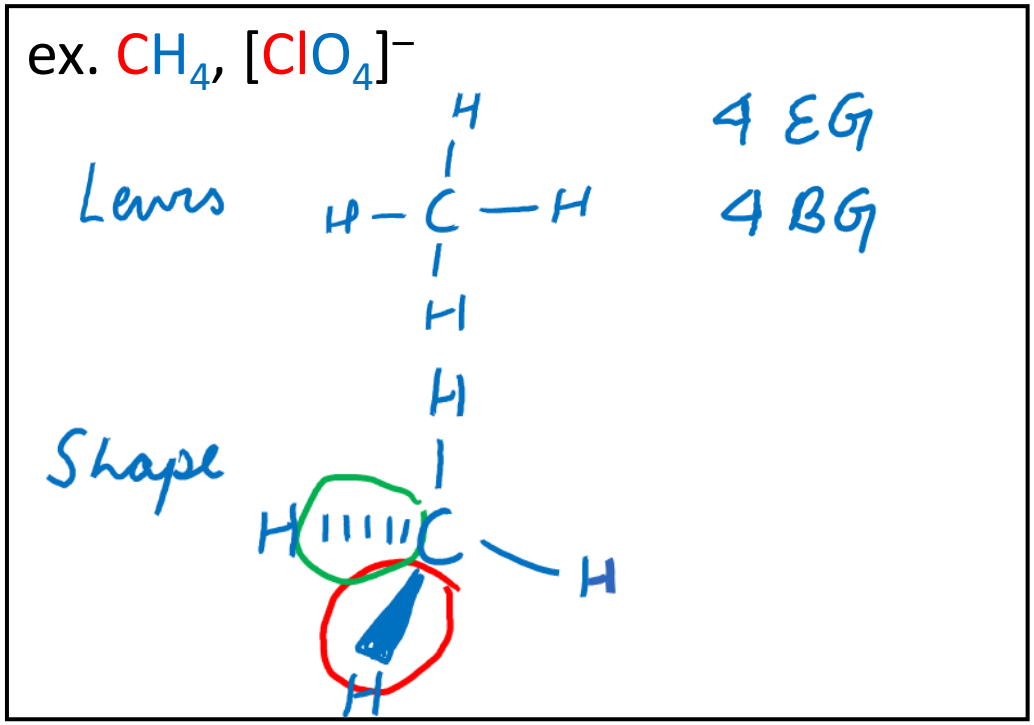
Molecule AX_4 (4 total electron groups)

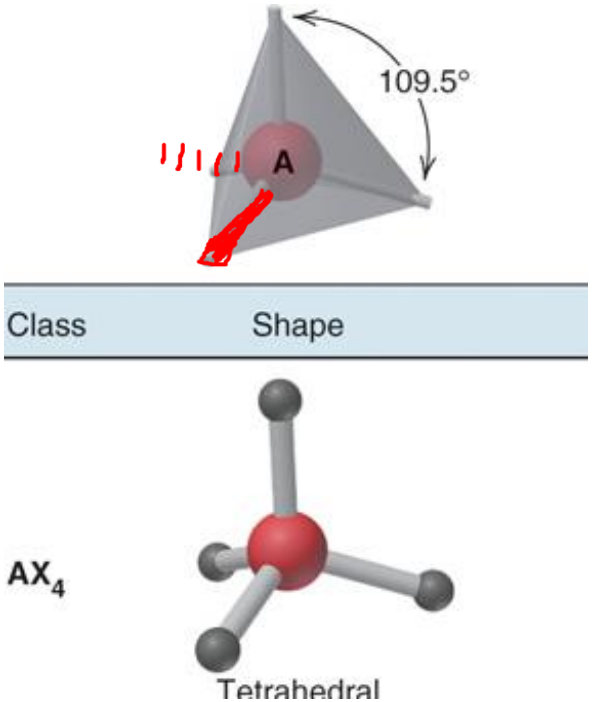
Tetrahedral Geometry (AX_4)

4 electron groups : 4 bonding groups (no lone pairs)

Bond Angle (XAX): 109.5 °

ex. CH_4, $[ClO_4]^-$





Molecule AX_3E (4 total electron groups)

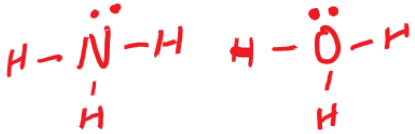
Trigonal Pyramidal Geometry (AX_3E)

4 electron groups : 3 bonding groups + 1 lone pair

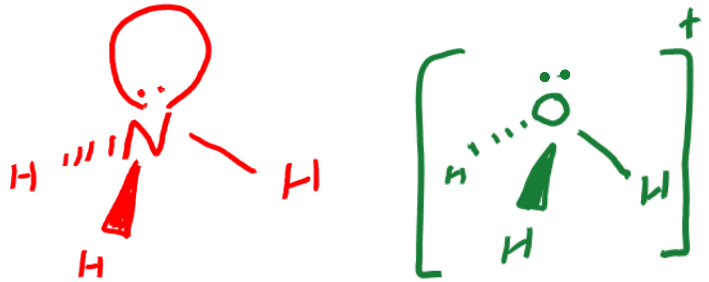
Bond Angle (XAX) < 109.5˚

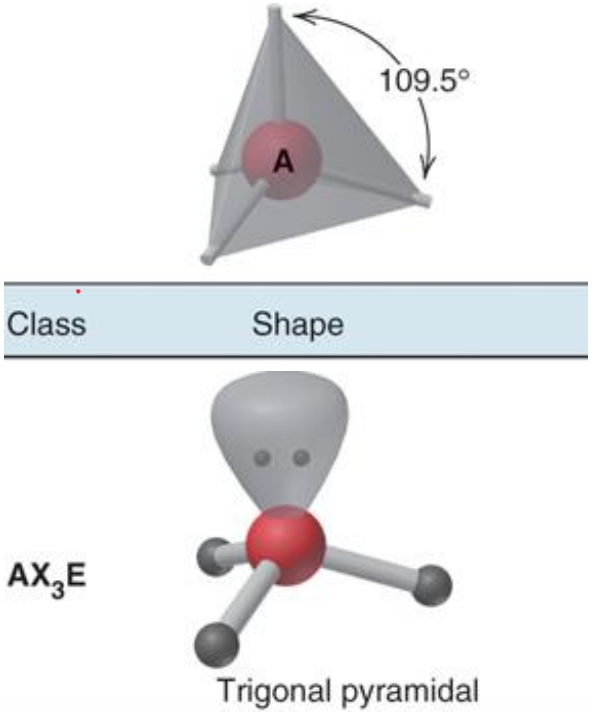
ex. NH_3, H_3O^+

Lewis



Shape





Molecule AX_2E_2 (4 total electron groups)

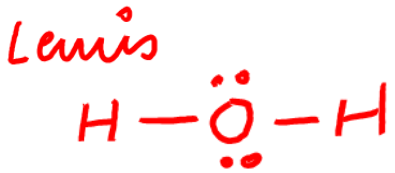
Bent Geometry (AX_2E_2)

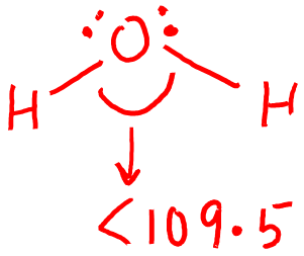
4 electron groups : 2 bonding groups + 2 lone pair

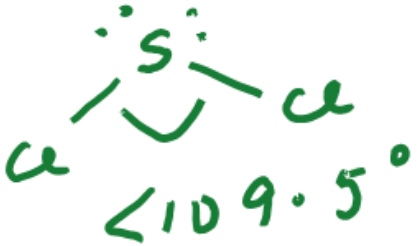
Bond Angle (XAX) < 109.5˚

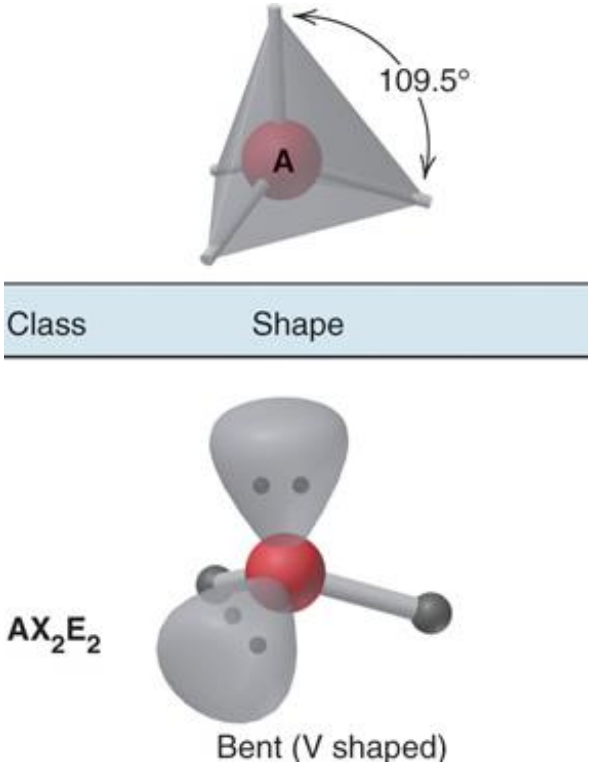
ex. H_2O, SCl_2

Lewis

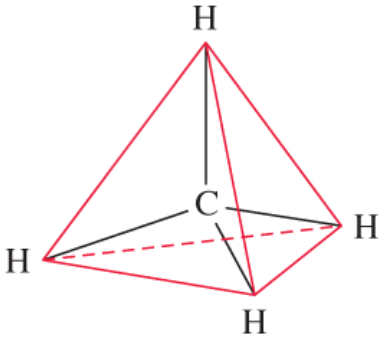


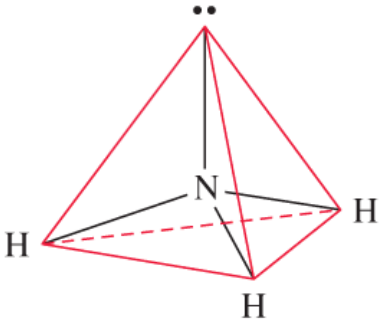


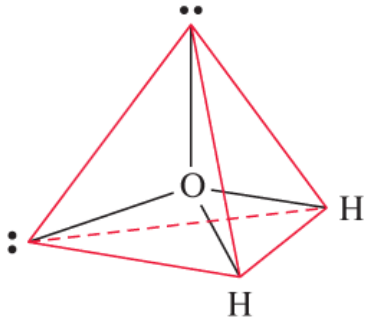


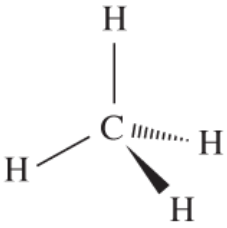


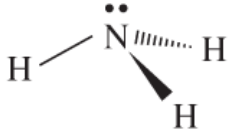
Drawing Tetrahedral Molecular Shapes

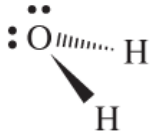












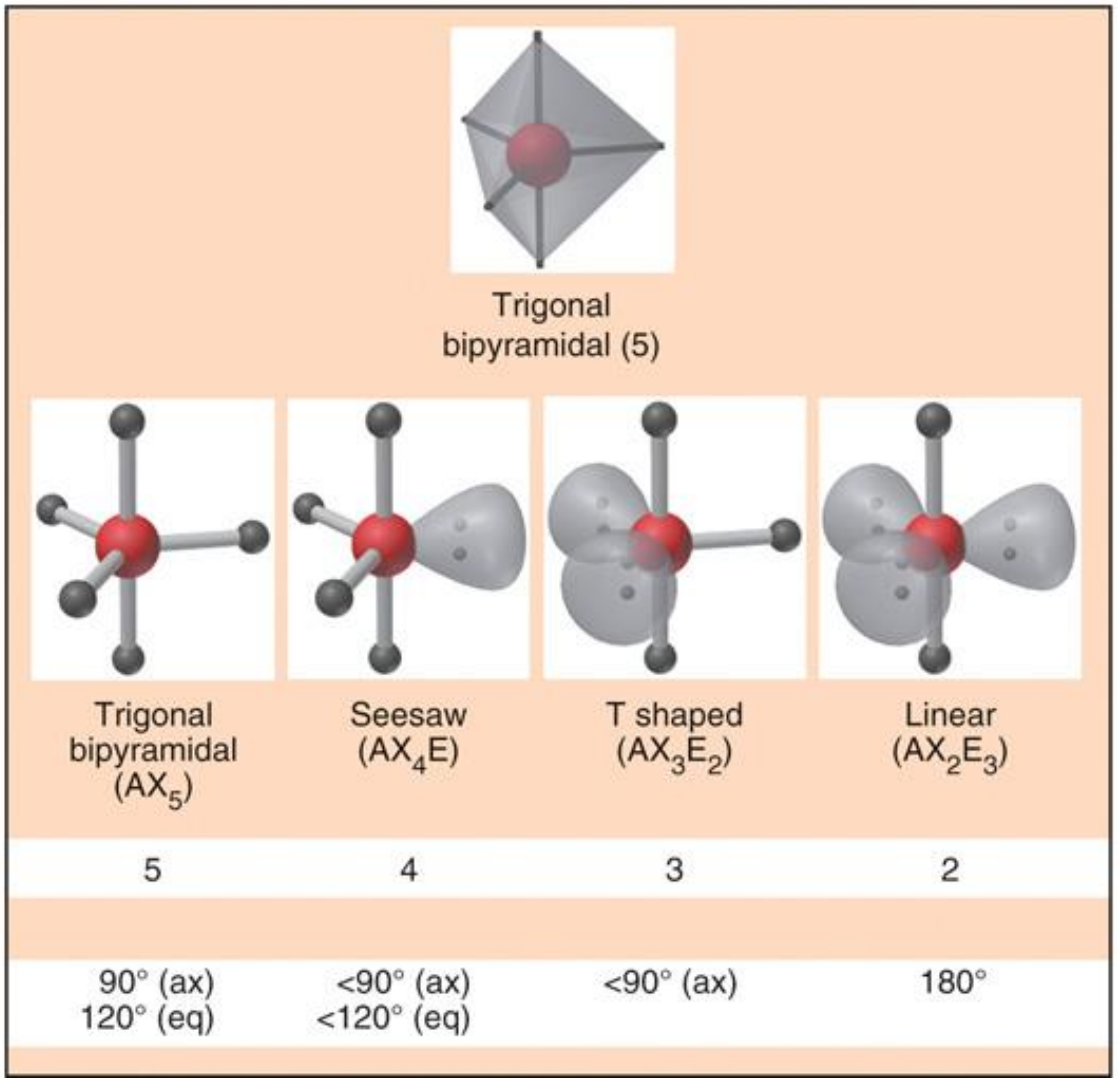
Molecular shape:	tetrahedral	trigonal pyramidal	bent
VSEPR notation:	AX_4	AX_3E	AX_2E_2

"wedge"  **"dash"** 

Molecular Geometry based on VSEPR

Continuing with different molecular shapes (more than 4 electron groups

Trigonal Bipyramidal(5 electron groups)

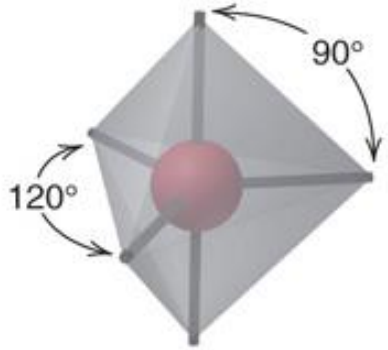


Molecule AX_5

Trigonal Bipyramidal (AX_5)

5 electron groups : 5 bonding groups (No lone pairs)

Bond Angles (XAX) : 120˚ and 90˚



Class	Shape
AX_5	Trigonal bipyramidal

Axial Bonds

Equatorial Bonds

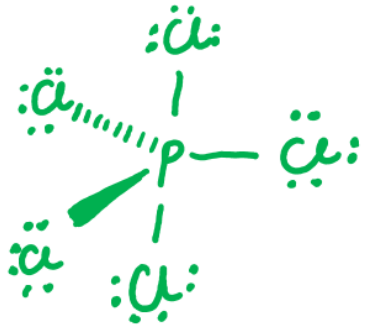
Molecule AX_5

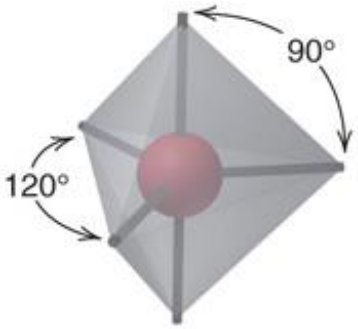
Trigonal Bipyramidal (AX_5)

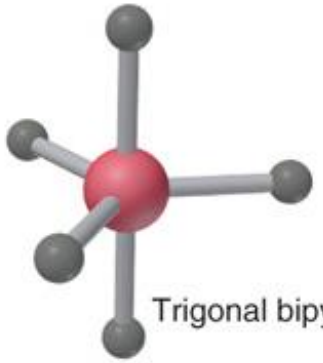
5 electron groups : 5 bonding groups (No lone pairs)

Bond Angles (XAX) : 120˚ and 90˚

ex. PCl_5, SOF_4





Class	Shape
AX_5	 Trigonal bipyramidal

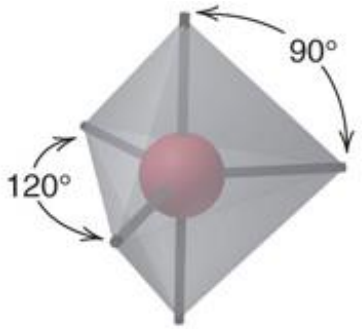
Molecule AX_4E

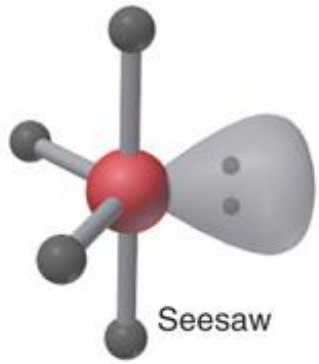
See-saw Geometry (AX_4E)

5 electron groups : 4 bonding groups + 1 lone pair

Bond Angles (XAX) : <120˚ and <90˚

ex. SF_4 Lewis



Class	Shape
AX_4E	

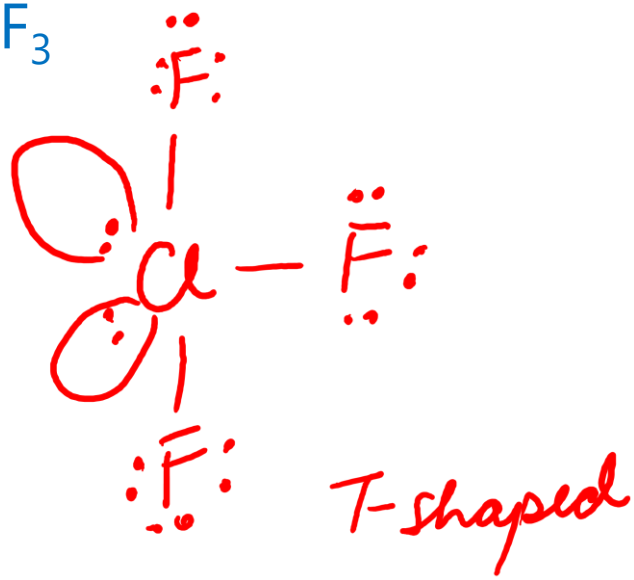
Molecule AX_3E_2

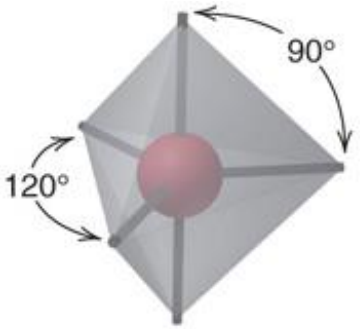
T-shaped Geometry (AX_3E_2)

5 electron groups : 3 bonding groups + 2 lone pairs

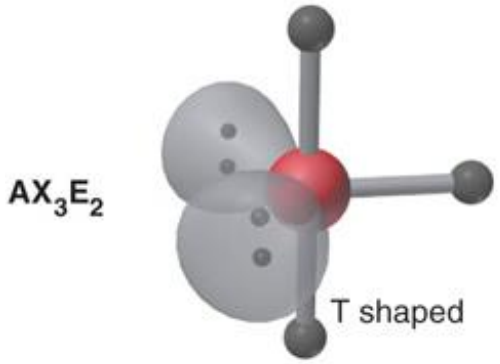
Bond Angles (XAX) : <90˚

ex. ClF_3





Class	Shape



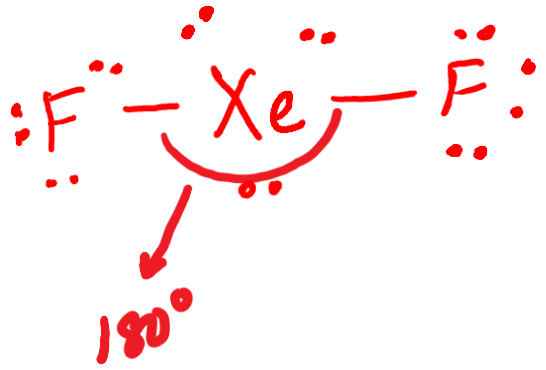
Molecule AX_2E_3

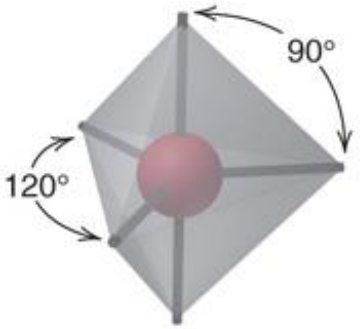
Linear Geometry (AX_2E_3)

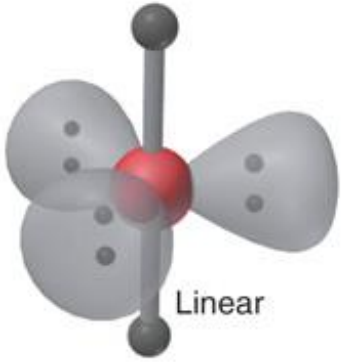
5 electron groups : 2 bonding groups + 3 lone pairs

Bond Angles (XAX) : 180˚

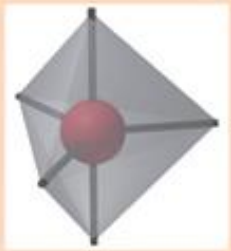
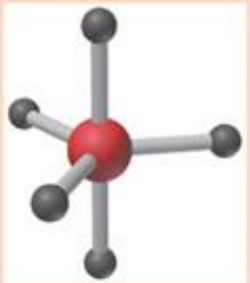
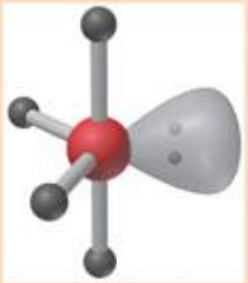
ex. XeF_2



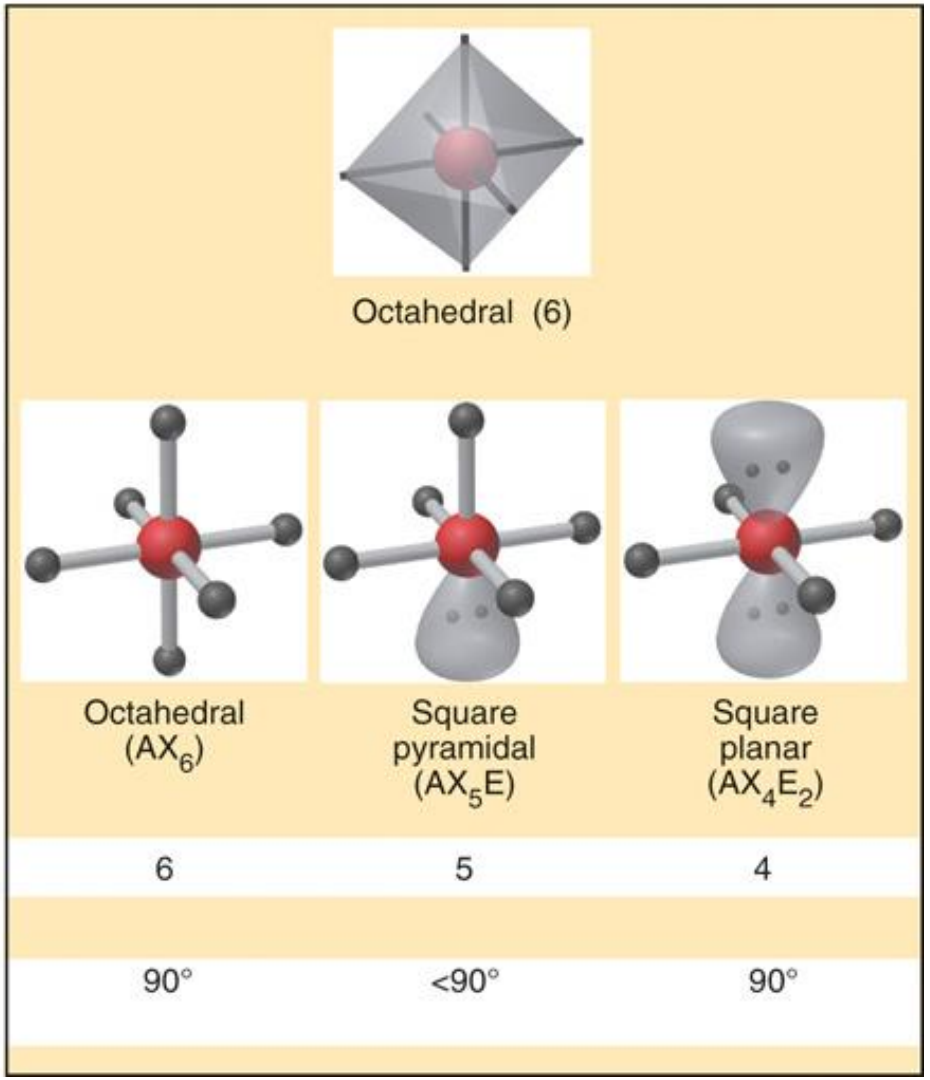


Class	Shape
AX_2E_3	

Trigonal Bipyramidal Summary

e^- Group arrangement (no. of groups)	 Trigonal bipyramidal (5)			
Molecular shape (class)	 Trigonal bipyramidal (AX_5)	 Seesaw (AX_4E)	 T shaped (AX_3E_2)	 Linear (AX_2E_3)
No. of bonding groups	5	4	3	2
Bond angle	90° (ax) 120° (eq)	<90° (ax) <120° (eq)	<90° (ax)	180°

Octahedral(Six electron groups)



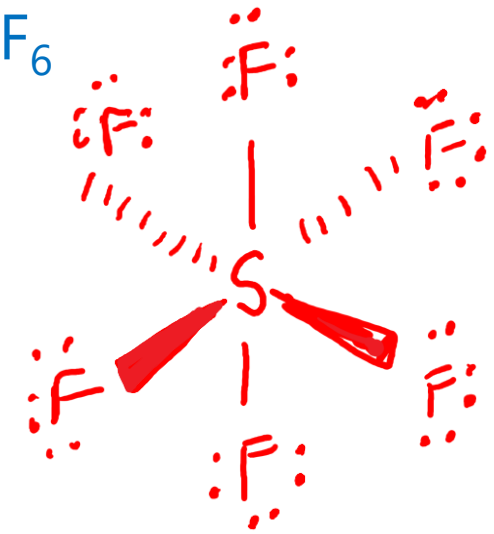
Molecule AX_6

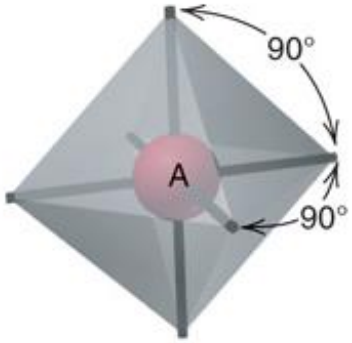
Octahedral Geometry (AX_6)

6 electron groups : 6 bonding groups

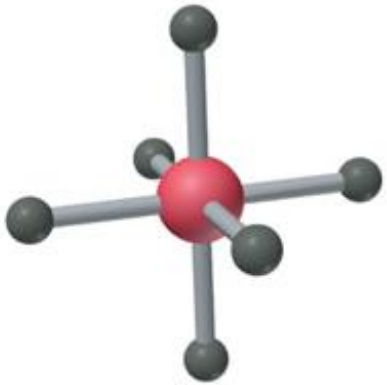
Bond Angles (XAX) : 90˚

ex. SF_6





Class	Shape
AX_6	Octahedral



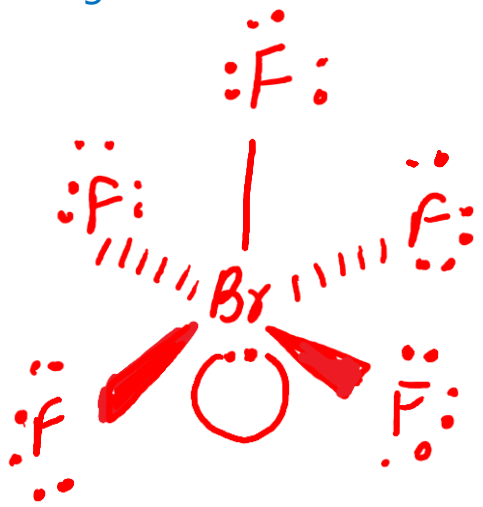
Molecule AX_5E

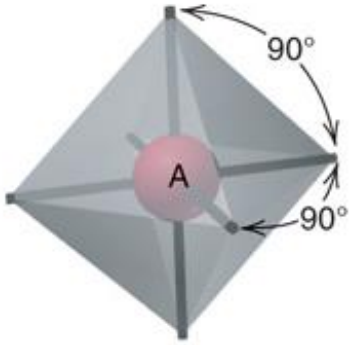
Square Pyramidal Geometry (AX_5E)

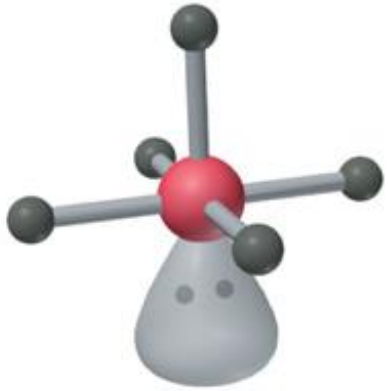
6 electron groups : 5 bonding groups + 1 lone pair

Bond Angles (XAX) : <90˚

ex. BrF_5





Class	Shape
AX_5E	

Square pyramidal

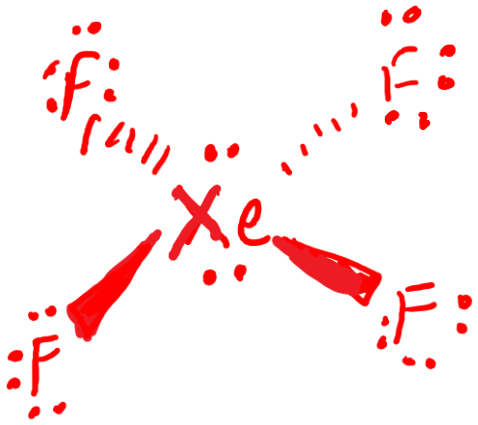
Molecule AX_4E_2

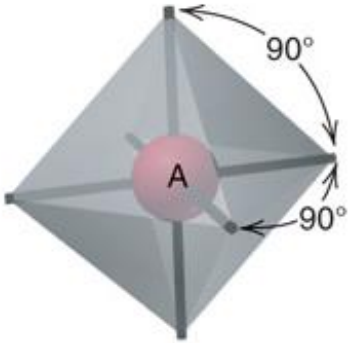
Square Planar Geometry (AX_4E_2)

6 electron groups : 4 bonding groups + 2 lone pairs

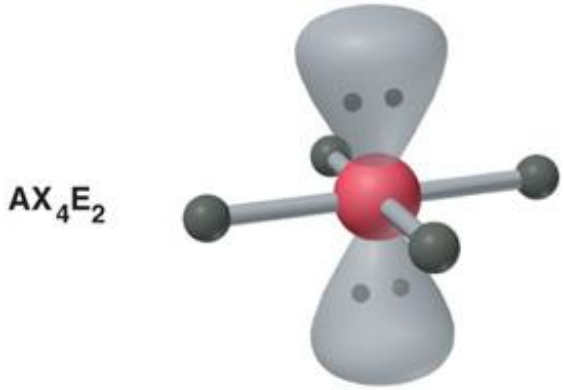
Bond Angles (XAX) : 90˚

ex. XeF_4



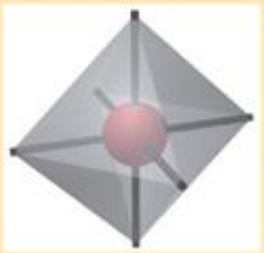
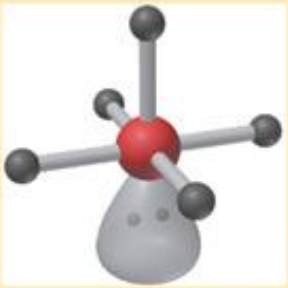
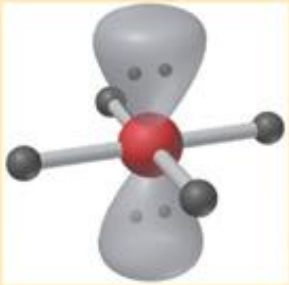


Class	Shape



Square planar

Octahedral Summary

e^- Group arrangement (no. of groups)	 Octahedral (6)		
Molecular shape (class)	 Octahedral (AX_6)	 Square pyramidal (AX_5E)	 Square planar (AX_4E_2)
No. of bonding groups	6	5	4
Bond angle	90°	<90°	90°

Determining Polarity of Molecules Based on Geometry

Based on the difference in χ (**Δχ**) between two atoms a **bond** can be described as polar (unequal sharing of electrons) or non-polar

		Δχ
Polar		
H—F	2.1 4.0	1.9
Non-Polar		
H—CH_3	2.1 2.5	0.4
Non-Polar		
Cl—Cl	3.0 3.0	0

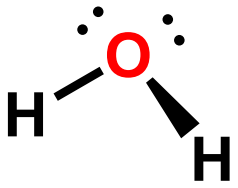
Usually polar covalent bonds are between atoms with Δχ = 0.5 – 1.9
High difference in electronegativity between the atoms leads to unequal sharing of electron pair.

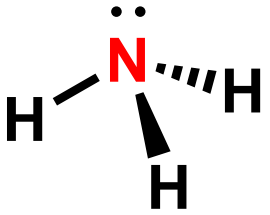
Determining Polarity of Molecules Based on Geometry

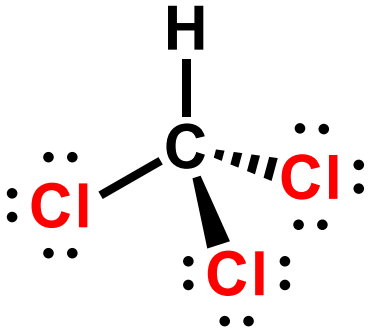
Based on the difference in χ (**Δχ**) between two atoms a **bond** can be described as polar (unequal sharing of electrons) or non-polar

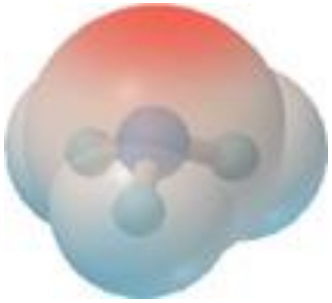
POLAR MOLECULES: molecules with a net dipole moment (μ)

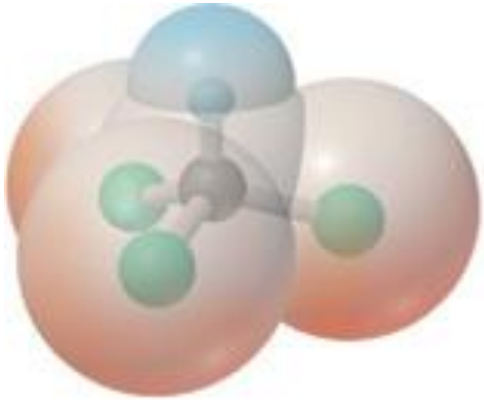
* "add up" the individual bond dipoles *











Determining Polarity of Molecules Based on Geometry

Based on the difference in χ (**Δχ**) between two atoms a **bond** can be described as polar (unequal sharing of electrons) or non-polar

NONPOLAR MOLECULES: molecules with **zero** net dipole moment (μ)
Either no individual bond dipoles or the individual bond dipoles cancel out