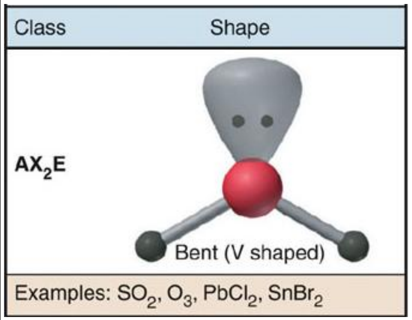
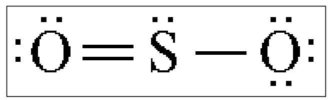
- **Trigonal planar** electron-group arrangement with **one lone pair**

→**Two** atoms attached to the central atom + **one** lone pair (**AX_2E**) → **Bent shape**

→The **lone pair is bulkier** and repels the bonding pairs stronger → **bond angle is less than 120°**



Example: SO_2



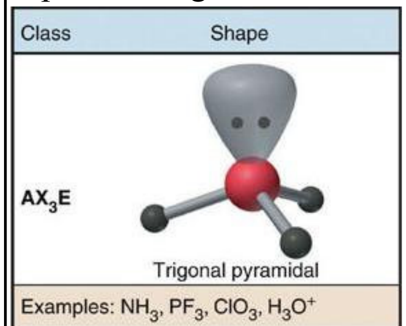
Bent shape

Bond angle of ~119°

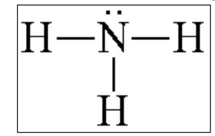
- **Tetrahedral** electron-group arrangement with **one lone pair**

→**Three** atoms attached to the central atom + **one** lone pair (**AX_3E**) → **Trigonal pyramidal shape**

→The **lone pair is bulkier** and repels the bonding pairs stronger → **bond angles are less than 109.5°**



Example: NH_3



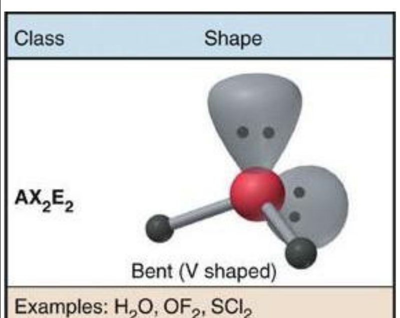
Trigonal pyramidal shape

Bond angle of 107.3°

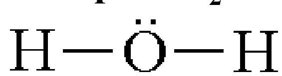
- **Tetrahedral** electron-group arrangement with **two lone pairs**

→**Two** atoms attached to the central atom + **two** lone pairs (**AX_2E_2**) → **Bent shape**

→The **two lone pairs** have even greater repelling effect → **bond angles are less than 109.5°**



Example: H_2O



Bent shape

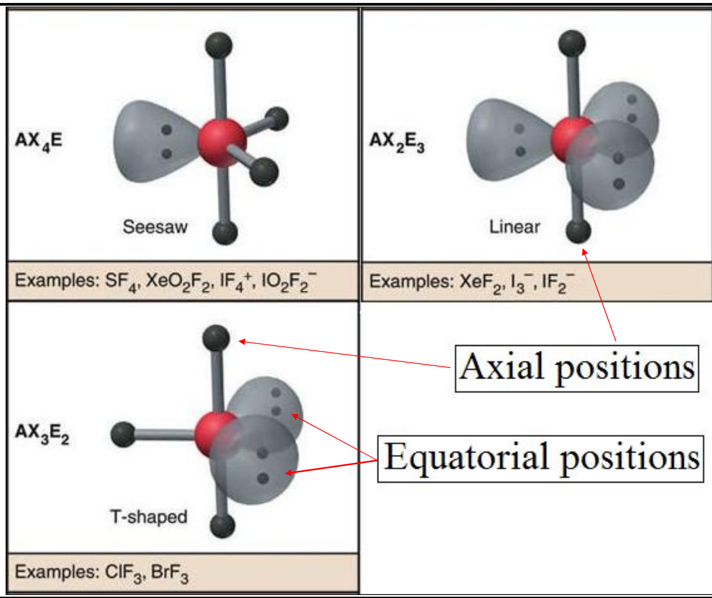
Bond angle of 104.5° (lower than in NH_3)

- Strengths of electron group repulsions

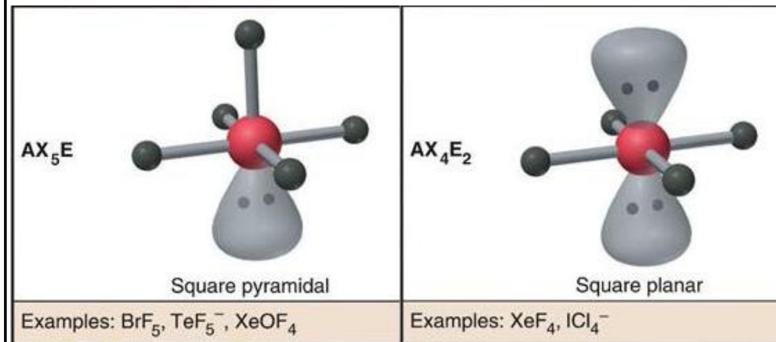
lone pair-lone pair > lone pair-bonding pair > bonding pair-bonding pair

⇒In the electron arrangement, lone pairs occupy positions as far from one another and from bonding pairs as possible

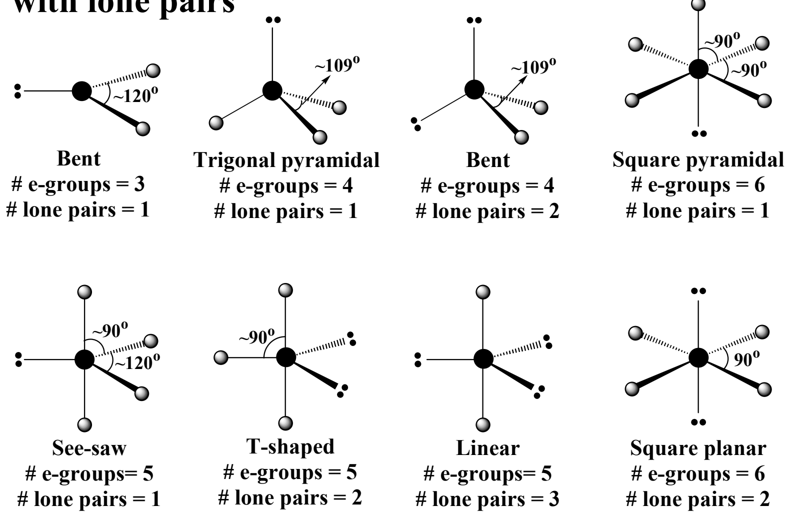
- **Trigonal bipyramidal** electron-group arrangement with **1**, **2** or **3 lone pairs**
  - VSEPR classes **AX_4E**, **AX_3E_2** and **AX_2E_3**
  - The **lone pairs occupy *equatorial* positions** (provides more space for the lone pairs and minimizes the repulsion)



- **Octahedral** electron-group arrangement with **1** or **2 lone pairs**
  - VSEPR classes $\mathbf{AX_5E}$, and $\mathbf{AX_4E_2}$
  - The **lone pairs occupy positions opposite to each other** (provides the lowest repulsion)



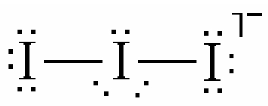
Summary of molecular shapes for central atoms with lone pairs



- **Steps** in determining molecular shapes using the VSEPR model:
  - Write the Lewis structure
  - Determine the electron-group arrangement, ideal bond angles and VSEPR class
  - Place the surrounding atoms and lone pairs in appropriate positions around the central atom and predict any deviations from the ideal bond angles
  - Name the molecular shape
- For molecules with **more than one central atom**, find the electron-group arrangement and corresponding shape around each central atom (one central atom at a time)

Example: Determine the electron arrangement and molecular shape of I_3^-.

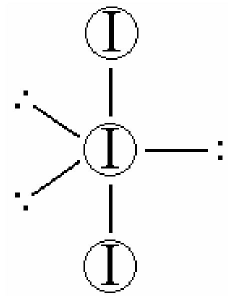
1. Lewis structure →



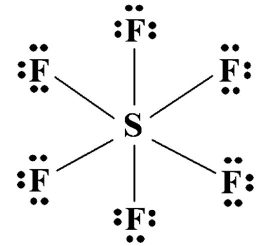
2. El-group arrangement → **trigonal bipyramidal** (**2** bonded atoms + **3** lone pairs = **5**), VSEPR class **AX_2E_3**

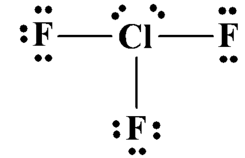
3. Lone pairs in equatorial positions, atoms in axial positions (**180°** bond angle)

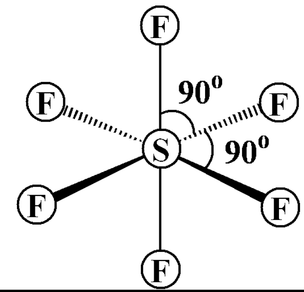
4. Molecular shape → **linear**

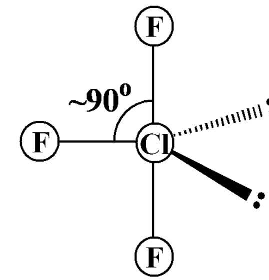


Example: Determine the shapes of **SF_6** and **ClF_3**









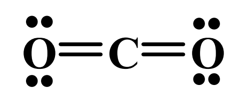
10.3 Charge Distribution in Molecules

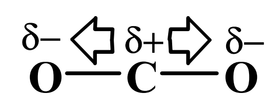
Bond Polarity and Molecular Polarity

- **Polar covalent bonds** (due to unequal sharing of the bonding electrons) → **bond dipoles**
- **Dipole moment** (μ) – a measure of the magnitude and direction of a dipole
  - μ increases with increasing the partial charges of the atoms (Q) and the bond distance (r) → $\mu = Q \cdot r$
  - The direction of μ is from plus to minus
  - SI units → **C·m**
  - Other units → **debye (D)** **1 D = 3.336×10^{-30} C·m**

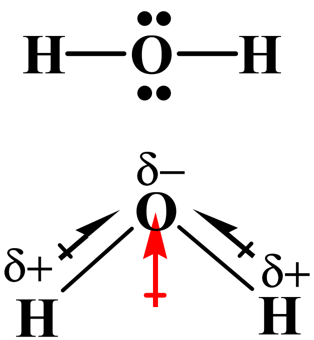
- **Molecular dipole moment** (associated with the molecule as a whole) – can be represented as a sum of the bond dipoles of all bonds
- **Nonpolar** molecules – zero dipole moment
  - Homonuclear diatomic molecules (**H_2**, **O_2**, **F_2**, ...)
  - Polyatomic molecules where the bond dipoles cancel each other

CO_2 is nonpolar – the bond dipoles of the **C–O** bonds cancel due to the linear shape





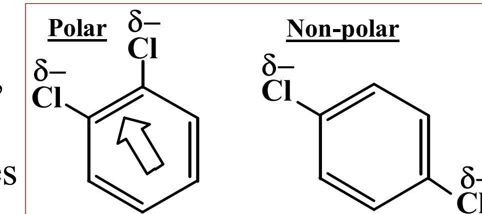
- **Polar** molecules – nonzero dipole moment
  - Heteronuclear diatomic molecules (**HF**, **CO**, ...)
  - Polyatomic molecules where the bond dipoles do not cancel each other



H_2O is a polar molecule because the bond dipoles of the O-H bonds do not cancel due to the bent molecular shape

⇒The polarity of molecules depends on both the polarity of the bonds and the molecular geometry which must be known

Example: The <u>isomers</u> 1,2-dichlorobenzene and 1,4-dichlorobenzene have the same formula, $C_6H_4Cl_2$, but different physical properties



B.p. 180°C Very soluble in EtOH

B.p. 174°C Slightly soluble in EtOH

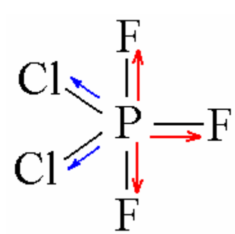
- Highly symmetric molecules are normally nonpolar
  - **AX_n** molecules (n=2, 3, 4, 5, 6) where **X** are atoms of the same element
  - Molecules with symmetrically positioned lone pairs (**AX_2E_3**, **AX_4E_2**)
- Molecules with asymmetrically positioned lone pairs or different atoms attached to the central atom are normally polar
  - **AX_2E**, **AX_2E_2**, **AX_3E**, **AX_3E_2**, **AX_4E**, **AX_5E**, …
  - **CF_3H**, **CF_2H_2**, **SO_2**(bent), ...

Example: Is **PCl_2F_3** a polar molecule?

1. The Lewis structure is similar to **PCl_5** (five atoms bonded to the **P** atom, no lone pairs)

⇒ **trigonal bipyramidal shape**

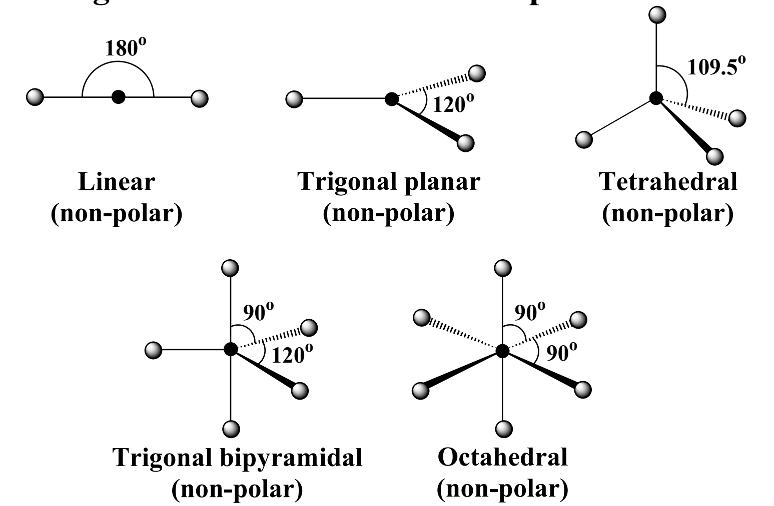
2. The **Cl** atoms are larger and take two of the equatorial positions; the **F** atoms are smaller and take the two axial and one of the equatorial positions



The **P–F** dipoles are larger than the **P–Cl** dipoles (*ΔEN* is larger for **P** and **F**)

The molecule is **polar** – the bond dipoles don't cancel (asymmetric arrangement)

Summary of molecular polarities for molecules having central atoms without lone pairs



Summary of molecular polarities for molecules having central atoms with lone pairs