MOLECULAR GEOMETRY (SHAPE)

- Molecular geometry of a molecule indicates the relative positions of its nuclei and can be determined experimentally.

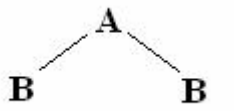
- Some molecules have very simple shapes:
  1. **All diatomic molecules are linear**

H — H Cl — Cl H — Cl N ≡ N

- Molecules containing more than 2 atoms may hypothetically have several different shapes.

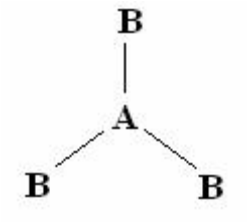
  2. **Triatomic molecules may have the following shapes**:

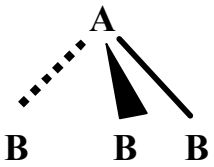
B — A — B **or**



Linear **Bent (or angular)**

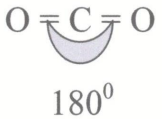
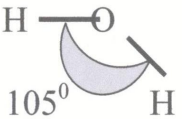
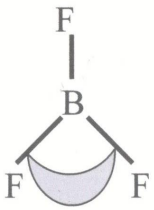
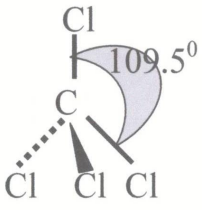
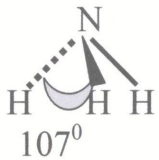
  3. **Tetraatomic molecules may have the following shapes**:





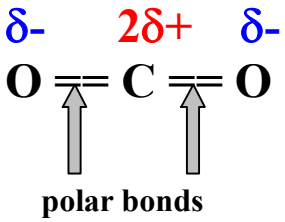
Trigonal planar **Trigonal pyramidal**

- Actual shapes of actual molecules are determined experimentally. Some examples of such shapes and their respective bond angles are given below:

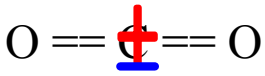
				
linear	bent (angular)	trigonal planar	tetrahedral	trigonal pyramidal

MOLECULAR POLARITY

- When a molecule contains more than two atoms bonded together it is possible to have a nonpolar molecule even though there are polar bonds present.
- In these molecules one must consider the molecular geometry (molecular shape) in order to decide if it is polar or not.

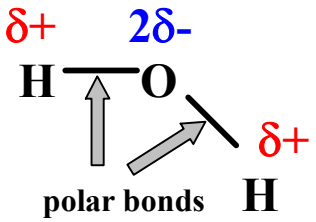


The **centers** of positive and negative charges **overlap**:

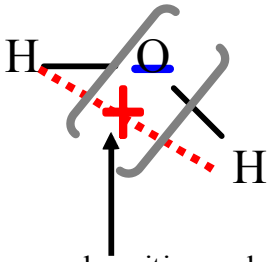


Electrical charges cancel

The **molecule** as a whole **is nonpolar**



The **centers** of positive and negative charges **do not overlap**:



dipole = equal positive and negative charges separated by a distance

Electrical charges do not cancel

The **molecule** as a whole **is polar** (is a dipole)

CONCLUSIONS

Molecular Polarity (polarity of the molecule as a whole) depends on

- **the polarity of the bonds and**
- **the molecular geometry (molecular shape)**

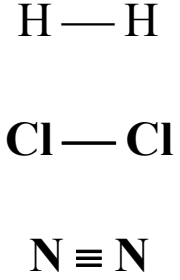
1. Molecules containing like atoms (nonpolar bonds) are nonpolar.

2. Molecules containing unlike atoms (polar bonds)

- **are NONPOLAR if the molecular shape is SYMMETRICAL**
- **are POLAR if the molecular shape is ASYMMETRICAL**

I. NONPOLAR MOLECULES

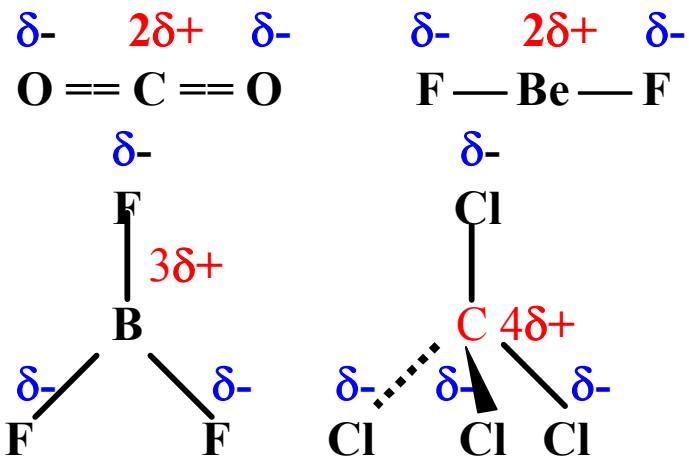
1. Contain like atoms



Nonpolar Bonds

Nonpolar Molecules

2. Contain unlike atoms in symmetrical arrangement



Centers of positive and negative charges overlap.

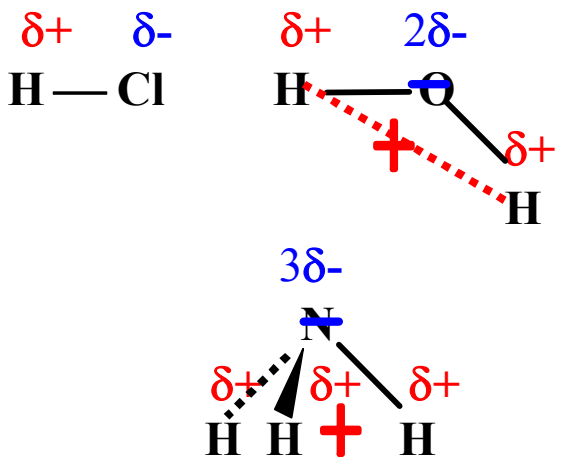
Electrical charges cancel

Polar Bonds

Nonpolar Molecules

II. POLAR MOLECULES

Contain unlike atoms in asymmetrical arrangement



Centers of positive and negative charges do not overlap.

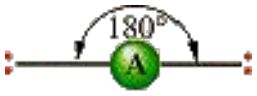
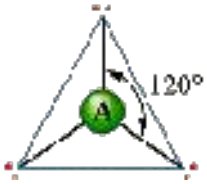
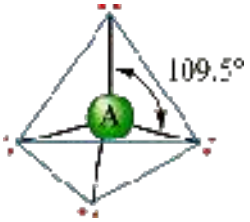
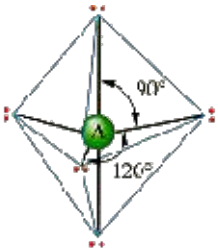
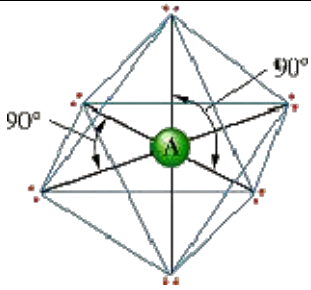
Electrical charges do not cancel

Polar Bonds

Polar Molecules (Dipoles)

VSEPR MODEL

- Chemists use several models to determine shapes of molecules.
- The simplest model is called VSEPR **(Valence Shell Electron Pair Repulsion Theory)**
- Based on this model, the electron pairs (both bonding and non-bonding) surrounding a central atom are positioned as far as possible form each other, thus minimizing electron-pair repulsions.

Number of Electron Pairs	Arrangement of Electron Pairs	Geometry of Molecule
2		Linerar
3		Trigonal Planar
4		Tetrahedral
5		Trigonal Bipyramidal
6		Octahedral