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Department of Chemistry

Topic

Valence Shell Electron Pair Repulsion Theory (VSEPER)

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❑ VSEPR-VALENCE SHELL ELECTRON PAIR REPULSION THEORY

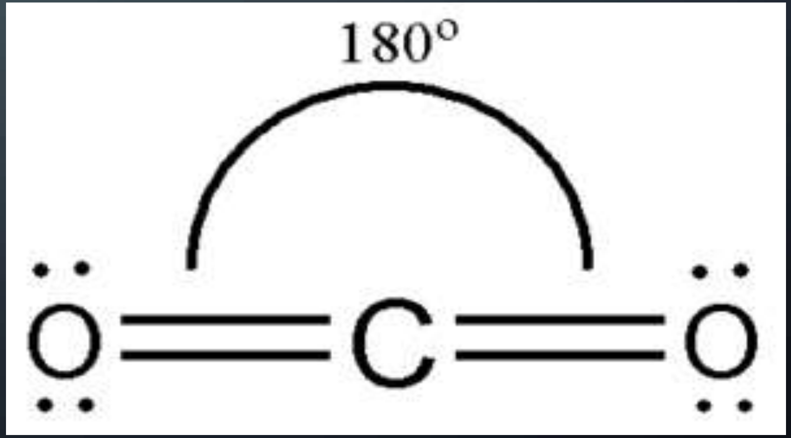
- The VSEPR Theory is used to predict the shape of the molecules from the electron

  pairs that surround the central atoms of molecule.
- The theory was first presented by Sidgwick and Powell in 1940.
- The VSEPR theory is based on the assumption that the molecule will take shape such that electron repulsion in the valence shell of that atom is minimised.
- Geometry of molecule depends upon the total number of valance shell electron pairs around the central atom.

❖ SHAPES OF SIMPLE INORGANIC MOLECULES AND IONS CONTANING LONE PAIRS

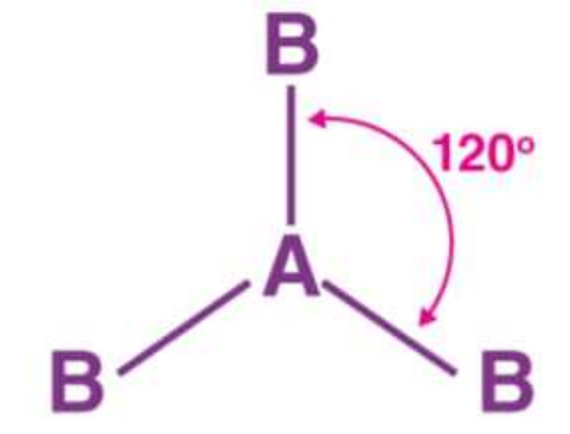
1. LINEAR:

- In this structure two molecules are attached to the centre atom. So they arranged in the opposite direction in order to minimize their repulsion.
- The bond angle of this structure is 180^o.
- 0 unshared pairs (lone pairs).
- Example: $BeCl_2$, $MgCl_2$, etc.
- Type : AX_2



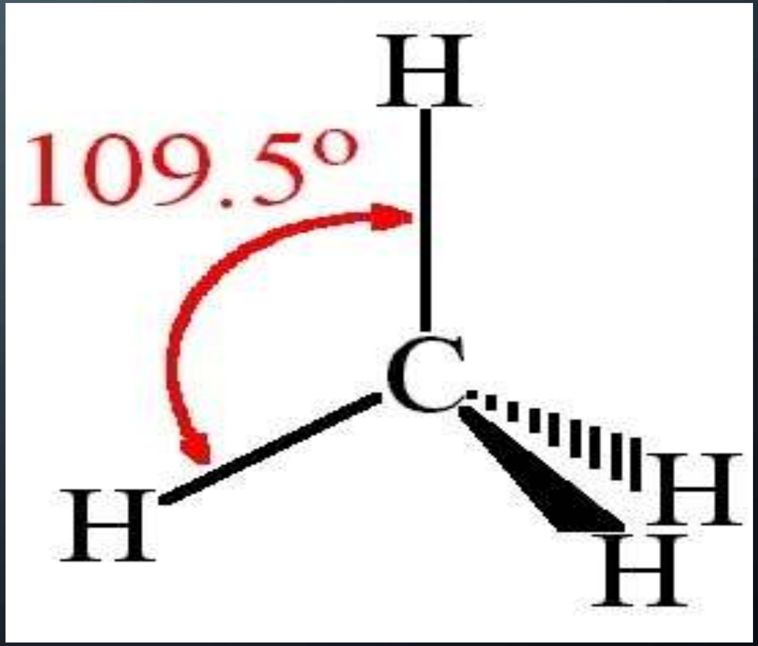
2.TRIGONAL PLANEAR

- In this type of molecule, we find three molecules attached to a central atom. So they are arranged towards the corners of an equilateral triangle in order to minimize their repulsion
- The bond angle of this structure is 120°.
- 0 lone pairs
- Example: BF_3, BCl_3, BBr_3 etc.
- Type : AX_3.



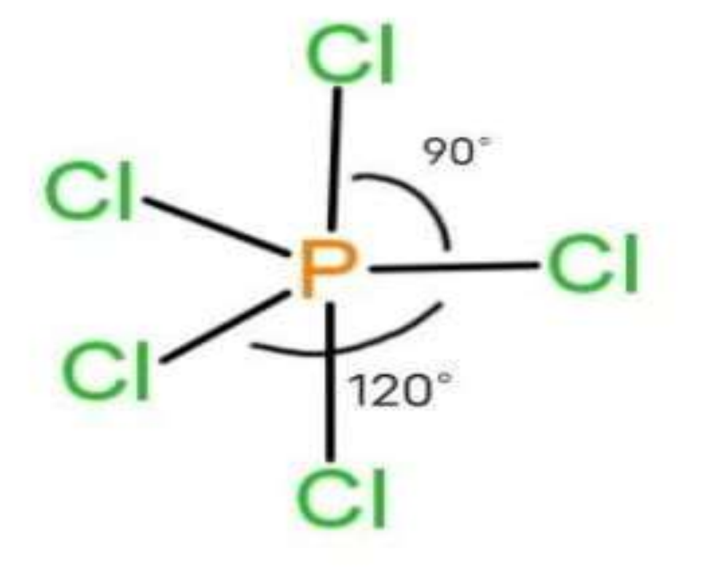
3. TETRAHEDRAL:

- In a tetrahedral molecular geometry, a central atom is located at the centre with four substituents that are located at the corners of a tetrahedron.
- The bond angle of the structure is 109.5°.
- 0 lone pairs.
- Example:CH4, CCl4 etc.
- Type :AX_4.



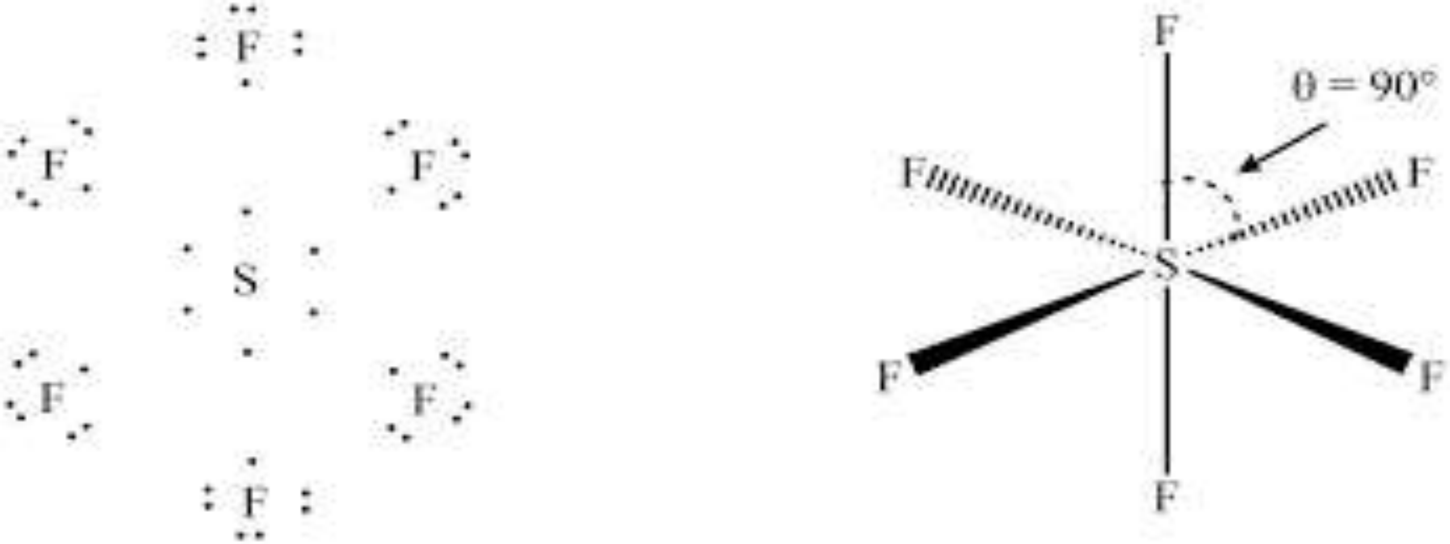
4.TRIGONAL BIPYRAMIDAL:

- Hear, repulsion can be minimized by even distribution of electron towards the corner of a trigonal pyramid. In a trigonal bipyramid, three positions lie along the equator of the molecule. The two positions lie along an axis perpendicular to the equatorial plane.
- The bond angle are 90° and120°.
- Type : AX_5.
- Example: PF_5 etc.



5. OCTAHEDRAL :

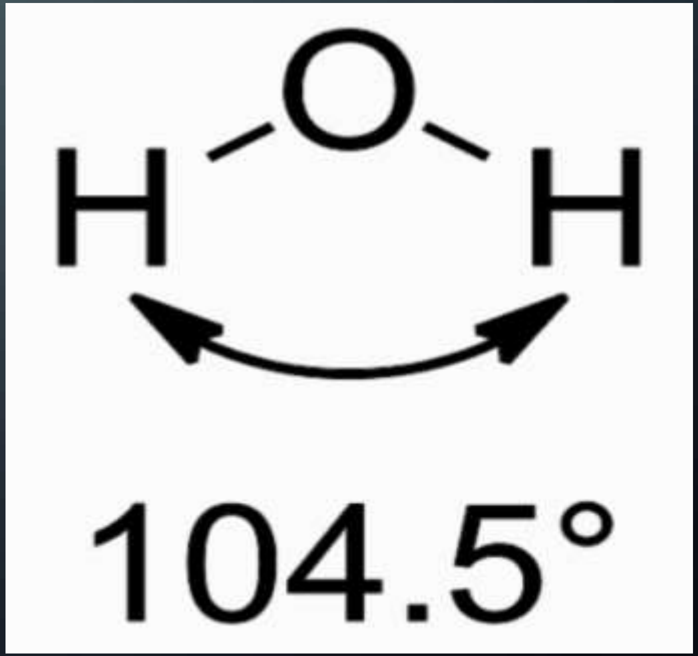
- Octahedral molecular geometry describes the shape of compounds with six atoms or groups of atoms or ligands symmetrically arranged around a central atom, defining the vertices of an octahedron.
- The bond angle is 90°.
- 0 lone pairs.
- Example: SF_6, TeF_6 etc.
- Type : SF_6



- ❑ **These are fore molecules with both paired and unshared (lone) pairs of electrons around the central atom.**

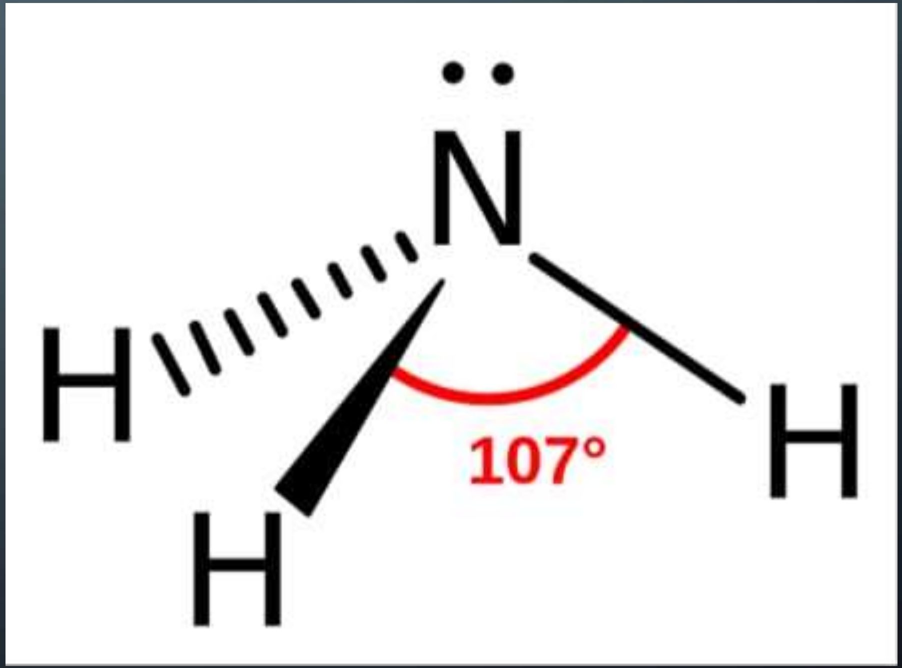
6. BENT

- ➢ Bant molecule is a kind of molecule in which the central atoms has two lone pairs of electron and associated with two bond pairs.
- ➢ It is also known as angular or v - shaped.
- ➢ The bond angle are 104.5^o.
- ➢ Type :AX_2E_2
- ➢ EX : H_2O



7. TRIGONAL PYRAMIDAL

- A trigonal pyramidal molecules have a central atom at the apex and three atoms at the corners of a trigonal base.
- The bond angle are 107^o.
- Type : AX_3E
- EX : NH_3

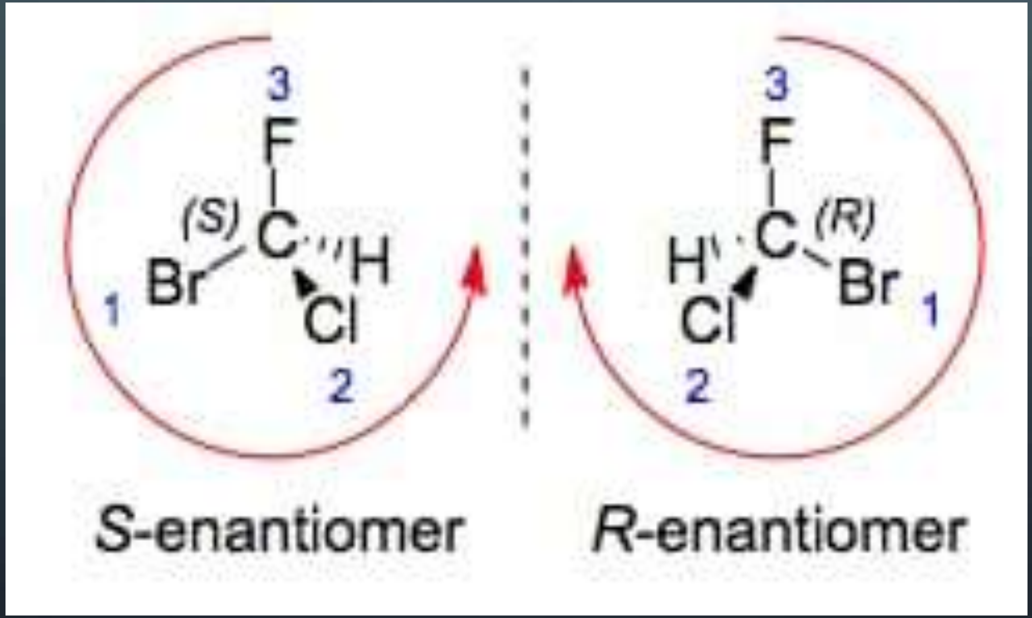


❖ STERIOCHEMISTRY RULS:

These rules are used to assign R or S to a chiral carbon atom.

1. Assign priorities to groups based on the atomic number of the first atom bonded to the chiral carbon.
2. Point the lowest priority group away from the viewer.
3. Number the remaining groups from highest to lowest priority.
4. Draw a circle starting at the highest priority group and ending at the lowest priority group with an arrow.

5. If the path traced is counterclockwise, the chiral central is assigned S.
6. If the path traced is clockwise, the chiral center is assigned R.



❖ RESULTANT GEOMETRY OF THE COMPOUND OF NON-TRANSITIONAL ELEMENTS

The geometry of compound of non-transition elements can be predicted by its coordination number, which determines the structure around the central atom.

- **Coordination number 3:** The geometry is trigonal planer, T shaped, or trigonal pyramidal.
- **Coordination number 4 :** The geometry is square planer , See Saw or tetrahedral.
- **Coordination number 5 :** The geometry is trigonal bipyramidal or square pyramidal.
- **Coordination number 6 :** The geometry is trigonal prism, hexagonal planer, octahedral.

- **Coordination number 7 :**The geometry is capped octahedral or capped trigonal prismatic.

- **Coordination number 8 :**The geometry is dodecahedral or bicapped trigonal prismatic or Square Antiprismatic.

- **Coordination number 9 :** The geometry is capped square antiprismatic.

In some octahedral and square planar complexes, cis and trans configurations are possible. Some octahedral complexes may also have optical isomers, which are mirror images that are not superimposable.

❑ APPLICATIONS OF VSEPR THEORY

- **Predicting molecular structure :** VSEPR theory can be used to predict the structure of molecules, such as the gaseous Co2 molecule.
- **Predicting Bond Angles:** VSEPR Theory can predict approximate bond angles By considering lone pair–lone pair, lone pair–bond pair, and bond pair–bond pair repulsions. Exa: CH_4 → 109.5°, NH_3 → ~107° & H_2O → ~104.5°
- **Predicting the number of high electron density regions:** VSEPR theory can be predict the number of high electron density regions around a central atom.
- **Predicting the structure of molecules with many bonds or unpaired electrons :** VSEPR theory can predict the structure of molecules or ions with many bonds or unpaired electrons.
- **Predicting the three-dimensional structure of compounds :** VSEPR theory can predict three-dimensional structure of many compounds with both metallic and non-metallic centres.
- **Predicting Molecular Polarity :** VSEPR Theory helps determine whether a molecule is **polar or non-polar.**

Exa: CO2 (Linear, Non – Polar) & H2O (Bent, Polar)

❖ LIMITATIONS OF VSEPR THEORY

- The structure of transition metal compounds and ions cannot be explained by the VSEPR theory.

- The isoelectronic species are not explained by VSEPR theory. Elements with the same amount of electrons are called isoelectronic species. Despite having the same number of electron isoelectronic species have different deviations and forms.

- The VSEPR hypothesis does not account for the effects of orbital interactions on molecule structures. As a result, actual molecule shapes are similar rather than exact to those anticipated by this theory.

- ✓Several compounds defy this idea since the theory ignores the active lone pairs and their corresponding substituent groups size.

- ✓According to this idea, the halves of Group 2 components should have a linear structure. However, their actual structure is a twisted one.

- ✓The exact bond angles between the atoms in a molecules cannot be determined using VSEPR theory.

- REFERENCE :-1) W. L. JOIIY : Modern Inorganic Chemistry
2) Puri, Sharma, Kaliya : Principle of Inorganic Chemistry

Thank you!