

Inorganic Chemistry/Chemical Bonding/VSEPR theory

Valence shell electron pair repulsion (VSEPR) theory (1957) is a model in chemistry, which is used for predicting the shapes of individual molecules, based upon their extent of electron-pair electrostatic repulsion, determined using steric numbers^[1]. The theory is also called the **Gillespie-Nyholm theory** after the two main developers. The premise of VSEPR is that a constructed Lewis structure is expanded to show all lone pairs of electrons alongside protruding and projecting bonds, for predicting the geometric shape and lone-pair behavior of a compound through consideration of the total coordination number.

VSEPR theory is based on the idea that the geometry of a molecule or polyatomic ion is determined primarily by repulsion among the pairs of electrons associated with a central atom. The pairs of electrons may be bonding or nonbonding (also called lone pairs). Only valence electrons of the central atom influence the molecular shape in a meaningful way.

Basic assumptions

1. Pairs of electrons in the valence shell of a central atom repel each other.
2. These pairs of electrons tend to occupy positions in space that minimize repulsions and maximize the distance of separation between them.
3. The valence shell is taken as a sphere with electron pairs localizing on the spherical surface at maximum distance from one another.
4. A multiple bond is treated as if it is a single electron pair and the two or three electron pairs of a multiple bond are treated as a single super pair.
5. Where two or more resonance structures can depict a molecule the VSEPR model is applicable to any such structure.

Three types of repulsion take place between the electrons of a molecule:

- The lone pair-lone pair repulsion
- The lone pair-bonding pair repulsion
- The bonding pair-bonding pair repulsion.

A molecule must avoid these repulsions to remain stable. When repulsion cannot be avoided, the *weaker repulsion* (i.e. the one that causes the smallest deviation from the ideal shape) is preferred.

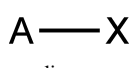
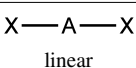
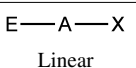
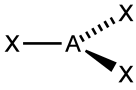
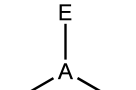
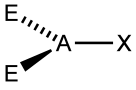
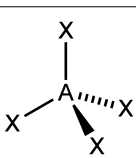
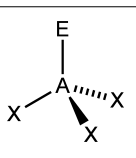
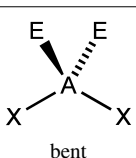
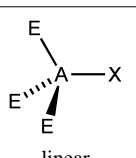
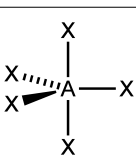
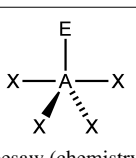
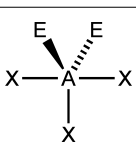
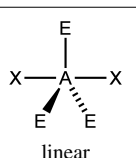
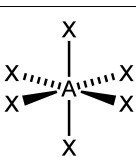
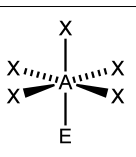
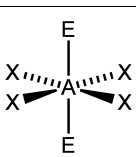
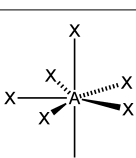
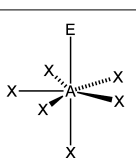
The lone pair-lone pair (lp-lp) repulsion is considered to be stronger than the lone pair-bonding pair (lp-bp) repulsion, which in turn is stronger than the bonding pair-bonding pair (bp-bp) repulsion. Hence, the weaker bp-bp repulsion is preferred over the lp-lp or lp-bp repulsion.





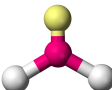
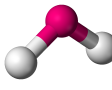
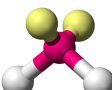
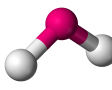
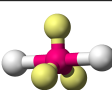
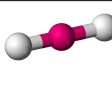
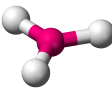
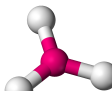
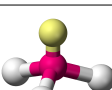
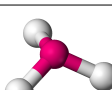
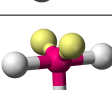
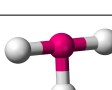
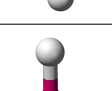
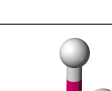
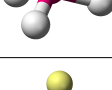
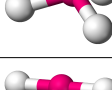
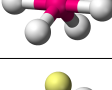
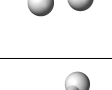
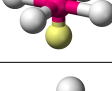
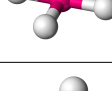
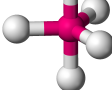
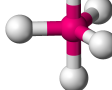
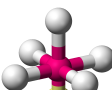
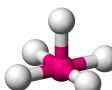
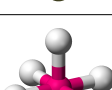
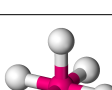
VSEPR theory is usually compared (but not part of) and contrasted with valence bond theory, which addresses molecular shape through orbitals that are energetically accessible for bonding. Valence bond theory concerns itself with the formation of sigma and pi bonds. Molecular orbital theory is another model for understanding how atoms and electrons are assembled into molecules and polyatomic ions.

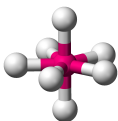
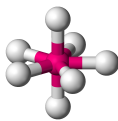
VSEPR theory has long been criticized for not being quantitative, and therefore limited to the generation of "crude", even though structurally accurate, molecular geometries of covalent molecules. However, molecular mechanics force fields based on VSEPR have also been developed.^[2]

AXE Method

The "AXE method" of electron counting is commonly used when applying the VSEPR theory. The *A* represents the central atom and always has an implied subscript one. The *X* represents how many sigma bonds are formed between the central atoms and outside atoms. Multiple covalent bonds (double, triple, etc) count as one *X*. The *E* represents the number of lone electron *pairs* present outside of the central atom. The sum of *X* and *E*, sometimes known as the steric number, is also associated with the total number of hybridised orbitals used by valence bond theory.

| Steric No. | Basic Geometry 0 lone pair | 1 lone pair | 2 lone pairs | 3 lone pairs |
|------------|---|---|--|---|
| 1 |  linear | | | |
| 2 |  linear |  Linear | | |
| 3 |  trigonal planar |  bent |  Trigonal Planar | |
| 4 |  tetrahedral |  trigonal pyramid |  bent |  linear |
| 5 |  trigonal bipyramid |  seesaw (chemistry) |  T-shaped (chemistry) |  linear |
| 6 |  octahedral |  square pyramid |  square planar | |
| 7 |  Pentagonal bipyramid |  pentagonal pyramid | | |

| Type | Shape | Geometry [†] | Geometry [‡] | Examples |
|-----------|----------------------|---|---|---|
| AX_1E_* | Diatomic |  |  | HF, O ₂ |
| AX_2E_0 | Linear |  |  | BeCl ₂ , HgCl ₂ , CO ₂ |
| AX_2E_1 | Bent |  |  | NO ₂ ⁻ , SO ₂ , O ₃ |
| AX_2E_2 | Bent |  |  | H ₂ O, OF ₂ |
| AX_2E_3 | Linear |  |  | XeF ₂ , I ₃ ⁻ |
| AX_3E_0 | Trigonal planar |  |  | BF ₃ , CO ₃ ²⁻ , NO ₃ ⁻ , SO ₃ |
| AX_3E_1 | Trigonal pyramidal |  |  | NH ₃ , PCl ₃ |
| AX_3E_2 | T-shaped |  |  | ClF ₃ , BrF ₃ |
| AX_4E_0 | Tetrahedral |  |  | CH ₄ , PO ₄ ³⁻ , SO ₄ ²⁻ , ClO ₄ ⁻ |
| AX_4E_1 | Seesaw |  |  | SF ₄ |
| AX_4E_2 | Square Planar |  |  | XeF ₄ |
| AX_5E_0 | Trigonal Bipyramidal |  |  | PCl ₅ |
| AX_5E_1 | Square Pyramidal |  |  | ClF ₅ , BrF ₅ |
| AX_6E_0 | Octahedral |  |  | SF ₆ |
| AX_6E_1 | Pentagonal pyramidal |  |  | XeF ₆ |

| | | | | |
|-----------|------------------------|---|---|--------|
| AX_7E_0 | Pentagonal bipyramidal |  |  | IF_7 |
|-----------|------------------------|---|---|--------|

† Geometry including lone pairs, shown in pale yellow

‡ Geometry excluding lone pairs

When the substituent (X) atoms are not all the same, the geometry is still approximately valid, but the bond angles may be slightly different than the ones where all the outside atoms are the same. For example, the double-bond carbons in alkenes like C_2H_4 are AX_3E_0 , but the bond angles are not all exactly 120° . Similarly, $SOCl_2$ is AX_3E_1 , but because the X substituents are not identical, the XAX angles are not all equal.

Examples

The methane molecule (CH_4) is tetrahedral because there are four pairs of electrons. The four hydrogen atoms are positioned at the vertices of a tetrahedron, and the bond angle is $\cos^{-1}(-1/3) \approx 109^\circ 28'$. This is referred to as an AX_4 type of molecule. As mentioned above, A represents the central atom and X represents all of the outer atoms.

The ammonia molecule (NH_3) has three pairs of electrons involved in bonding, but there is a lone pair of electrons on the nitrogen atom. It is not bonded with another atom; however, it influences the overall shape through repulsions. As in methane above, there are four regions of electron density. Therefore, the overall orientation of the regions of electron density is tetrahedral. On the other hand, there are only three outer atoms. This is referred to as an AX_3E type molecule because the lone pair is represented by an E. The overall shape of the molecule is a trigonal pyramid because the lone pair is not "visible." The shape of a molecule is found from the relationship of the atoms even though it can be influenced by lone pairs of electrons.

A steric number of seven is possible, but it occurs in uncommon compounds such as iodine heptafluoride. The base geometry for this is pentagonal bipyramidal.

References

- [1] *Modern Inorganic Chemistry* W.L. Jolly ISBN 0-07-032760-2
 [2] VGS Box. *Journal of Molecular Modeling*, 1997, 3, 124-141.

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