

VSEPR-Theory

Valence **S**hell **E**lectron **P**air **R**epulsion Theory or **VSEPR** is used to determine the spatial arrangement of sigma bonding pairs and lone pairs around a central atom in a small covalent molecule or a covalently bonded ion.

VSEPR Theory: the pairs of electrons around a central atom (this includes all sigma bonding electrons and lone pairs) will arrange themselves in such a way as to minimize the electrostatic force of repulsion.

This means that the electron pairs will occupy region of space around the central atom as far as possible from all other pairs.

Lone pairs have slightly more repulsion ability than sigma bonding pairs, since the lone pair will have a greater electron density closer to the central atom.

Pi bonding electrons are not included in the VSEPR Theory because the electronic charge in pi electrons is to spread out to cause much repulsion with other electron pairs. Furthermore, pi bonds always surround a central sigma bond.

The base shape of a molecule is based on all sigma bonds and all lone pairs if present.

The **actual shape** of the molecule is based on the sigma bonds only. The actual shape will be the same as the **base shape**, if no lone pairs are present. The actual shape will be a truncation of the base shape if lone pairs are present.

the shape based on atoms

electron shape, includes lone pairs

sigma (σ) is a single bond or the first bond in a double or triple bond, (carbon framework)

pi (π) is the second bond in a double bond or the second and third bond in a triple bond you cannot have a pi before a central sigma bond. Pi surrounds the sigma bond... Pi bonds are identified and then ignored with respect to shape

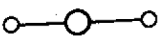
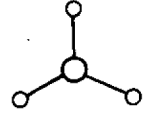
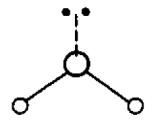
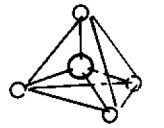
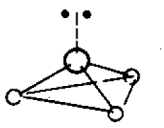
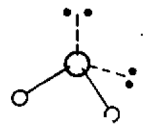
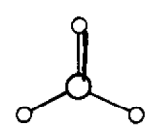
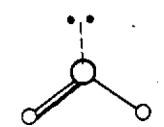
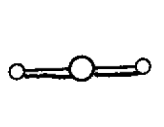
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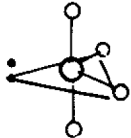
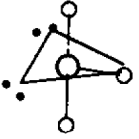
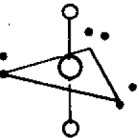
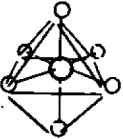
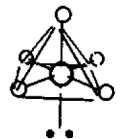
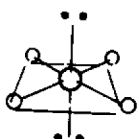
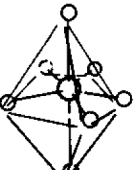
total electrons around "central" atom

σ bonding pair \leftarrow DETERMINE SHAPE

σ lone pair \leftarrow

π bonding pair - do not affect shape

Electron Pairs				Structure	Base Shape	Actual Shape	Bond Angle	Example
total	σ	lone	π					
2	2	0	0		linear	linear	180	BeF ₂
3	3	0	0		trigonal planar	trigonal planar	120	BF ₃
3	2	1	0		trigonal planar	angular	<120	SnCl ₂
4	4	0	0		tetrahedral	tetrahedral	109.5	CCl ₄
4	3	1	0		tetrahedral	pyramidal	<109.5	NH ₃
4	2	2	0		tetrahedral	angular	<109.5	H ₂ O
4	3	0	1		trigonal planar	trigonal planar	120	SO ₃
4	2	1	1		trigonal planar	angular	<120	SO ₂
4	2	0	2		linear	linear	180	CO ₂

Electron Pairs				Structure	Base Shape	Actual Shape	Bond Angle	Example
t o t a l	σ	l o n e	π					
5	5	0	0		trigonal bipyramidal	trigonal bipyramidal	90, 120	PCl_5
5	4	1	0		trigonal bipyramidal	seesaw	<90, <120	SF_4
5	3	2	0		trigonal bipyramidal	T-shaped	<90,	ClF_3
5	2	3	0		trigonal bipyramidal	linear	180	XeF_2
6	6	0	0		octahedral	octahedral	90	SF_6
6	5	1	0		octahedral	square based pyramid	<90	IF_5
6	4	2	0		octahedral	square planar	90	XeF_4
7	7	0	0		pentagonal bipyramid	pentagonal bipyramid	90, 72	IF_7