VSEPR-Theory

 $\underline{\mathbf{V}}$ alence $\underline{\mathbf{S}}$ hell $\underline{\mathbf{E}}$ lectron $\underline{\mathbf{P}}$ air $\underline{\mathbf{R}}$ epulsion Theory or $\underline{\mathbf{VSEPR}}$ 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 is such a away 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.

E	Electron Pairs						Angle	Example
t o t a 1	δ	l o n e	п	Structure	Base Shape	Actual Shape	Bond Ar	Ехап
2	2	0	0	o—o—o	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	$ m NH_3$
4	2	2	0		tetrahedral	angular	<109.5	H ₂ O
4	3	0	1		trigonal planar	trigonal planar	120	SO₃
4	2	1	1		trigonal planar	angular	<120	SO ₂
14	2	0	2	~	linear	linear	180	CO ₂

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σ		l				Angle	ub]
	n e	п	Structure	Base Shape	Actual Shape	Bond A	Example
5	0	0		trigonal bipyramidal	trigonal bipyramidal	90, 120	PCl ₅
4	1	0		trigonal bipyramidal	seesaw	<90, <120	SF ₄
3	2	0	.29	trigonal bipyramidal	T-shaped	<90,	ClF ₃
2	3	0		trigonal bipyramidal	linear	180	XeF ₂
6	0	0		octahedral	octahedral	90	\mathtt{SF}_6
5	1	0		octahedral	square based pyramid	<90	IF ₅
4	2	0		octahedral	square planar	90	XeF ₄
7	0	0		pentagonal bipyramid	pentagonal bipyramid	90, 72	IF ₇
	3 2 6 4	3 2 3 6 0 5 1 4 2	4 1 0 3 2 0 6 0 0 5 1 0 4 2 0	4 1 0 3 2 0 2 3 0 6 0 0 5 1 0 4 2 0	trigonal bipyramidal 4 1 0 trigonal bipyramidal 3 2 0 trigonal bipyramidal 2 3 0 trigonal bipyramidal 6 0 0 o octahedral 5 1 0 octahedral 4 2 0 pentagonal	trigonal bipyramidal trigonal bipyramidal trigonal bipyramidal trigonal bipyramidal trigonal bipyramidal T-shaped trigonal bipyramidal T-shaped trigonal bipyramidal Tous a cotahedral trigonal bipyramidal trigonal bipyramidal trigonal bipyramidal trigonal bipyramidal cotahedral cotahedral octahedral square based pyramid trigonal bipyramidal trigonal bipyramidal Tous a cotahedral octahedral square based pyramid octahedral square planar pentagonal pentagonal	trigonal bipyramidal 90, 120 trigonal bipyramidal seesaw <90, <120 trigonal bipyramidal T-shaped <90, <120 trigonal bipyramidal T-shaped <90, <120 trigonal bipyramidal Iinear 180 trigonal bipyramidal 0 ctahedral 90 octahedral octahedral 90 trigonal bipyramidal Iinear 180 octahedral square based pyramid <90 octahedral square planar 90 pentagonal pentagonal 90, 72