VSEPR & THE SHAPES OF MOLECULES

A SUMMARY OF THE MOLECULE SHAPES PREDICTED BY VALENCE SHELL ELECTRON PAIR REPULSION THEORY

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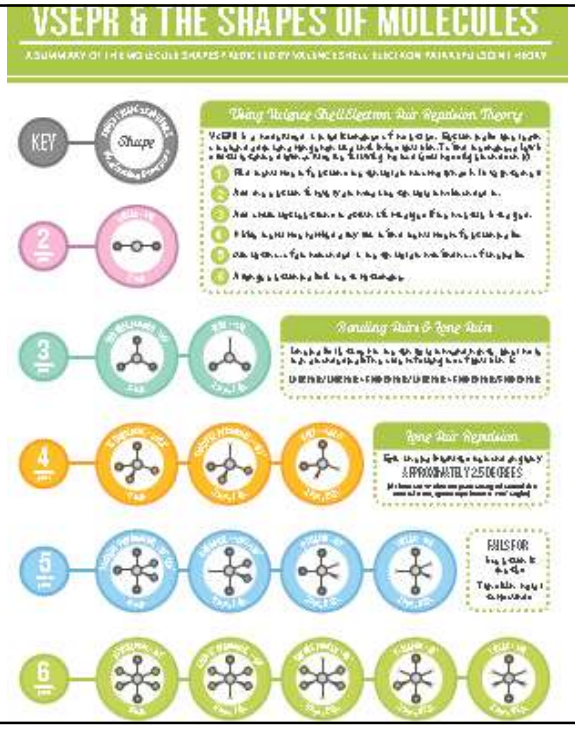

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VSEPR is a model used to predict shapes of molecules. Electron pairs repel each other, and adopt an arrangement that minimises repulsion.

To find the shape, a Lewis structure can be drawn, or use the following method (be careful with multiple bonds)

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3

Predict the shape of carbon tetrabromide, CBr_4.

❑ 1 Find the number of electrons the central atom normally has in its valence shell.
❑ 2 Add one electron for every atom that the central atom is bonded to. *

Carbon is in Group 14, and has four valence electrons; σ-bonds to four Br atoms contribute a total of four electrons.

❑ 3 Add or subtract electrons to account for charges if the molecule is charged.

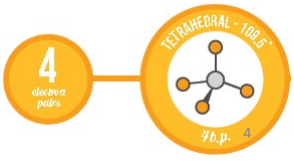
The central atom has no charge, so there are eight electrons (4 +4)

❑ 4 Divide the number arrived at by two to find the number of electron pairs.

$\frac{8}{2} = 4$ four pairs, on the carbon.

❑ 5 Subtract # of atoms bonded to the central atom electron pairs to find # of lone pairs.
4 Br atoms – 4 pairs bonded = 0 lone pairs

❑ 6 Arrange electron pairs in the correct shape (Table).
the shape is therefore a regular tetrahedron



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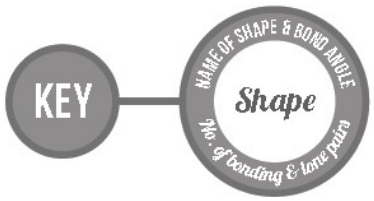
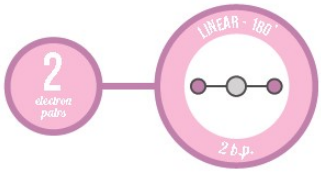


KEY: # Electron pairs

Name and Bond angle

 # bonded pairs, # lone pairs



Lineal, 180°

2 pairs

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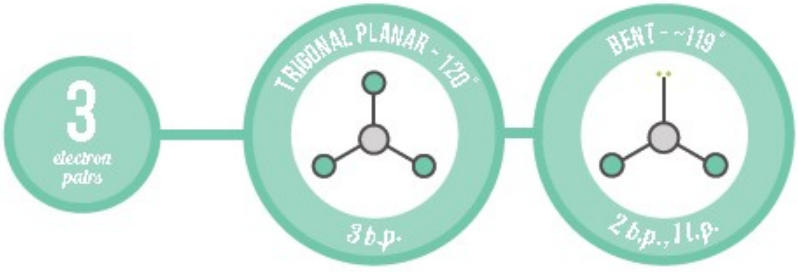

Trigonal planar, 120°

3 pairs

Angular, 119°

2 pairs, 1 lone pairs

Bonding Pairs & Lone Pairs

Lone pairs lie closer to the central atom, and hence repel more than a bonded pair.
The order of strengths of repulsion is:
LONE PAIR/LONE PAIR > BONDED PAIR/ LONE PAIR > BONDED PAIR/BONDED PAIR

6

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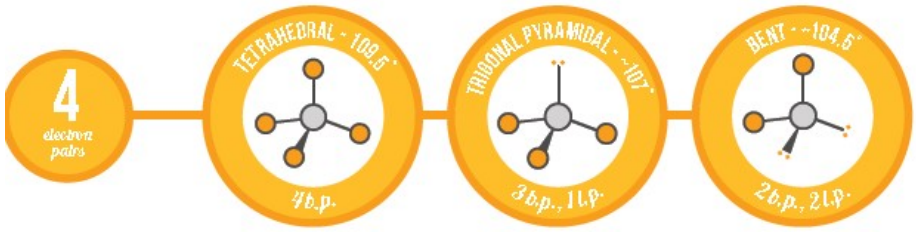

Td, 109.5°

4 pairs

Trig Pir, 107°

3 pairs, 1 lone p

Ang, 104.5°

2 pairs, 2 lone p

Lone Pair Repulsion

Each lone pair reduces the bond angle by APPROXIMATELY 2.5 DEGREES

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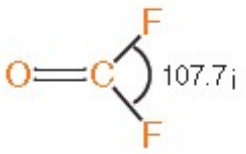
H_2O

COF_2



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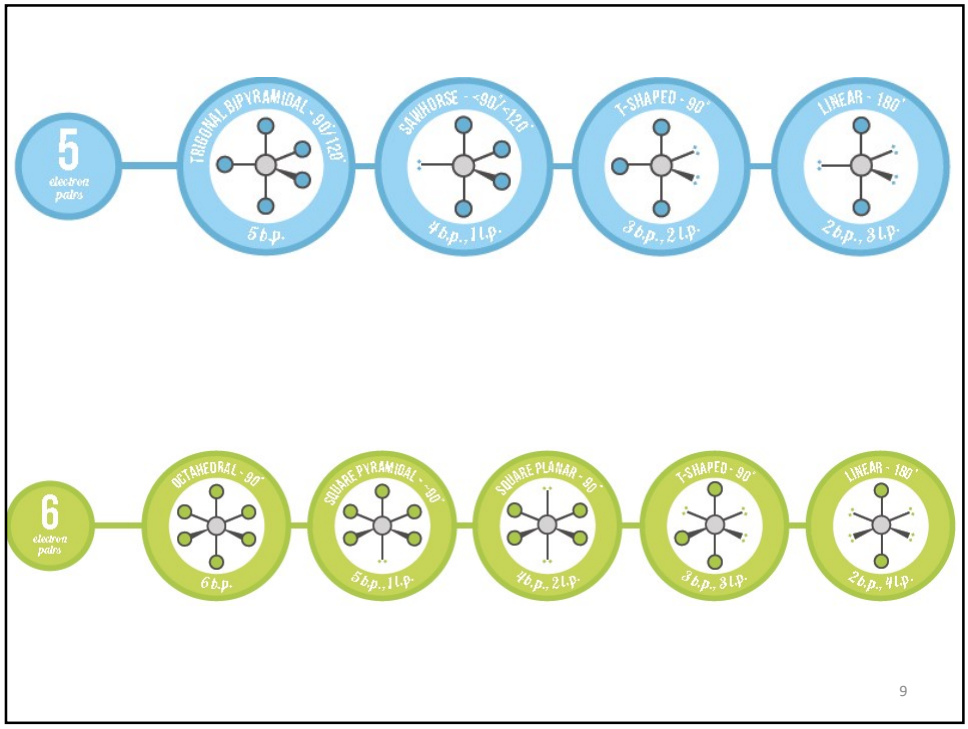
8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electron pairs
TRIGONAL BIPYRAMIDAL - 90°/120°
5 b.p.
SAWHORSE - <90°/<120°
4 b.p., 1 l.p.
T-SHAPED - 90°
3 b.p., 2 l.p.
LINEAR - 180°
2 b.p., 3 l.p.
6
electron pairs
OCTAHEDRAL - 90°
6 b.p.
SQUARE PYRAMIDAL - <90°
5 b.p., 1 l.p.
SQUARE PLANAR - 90°
4 b.p., 2 l.p.
T-SHAPED - 90°
3 b.p., 3 l.p.
LINEAR - 180°
2 b.p., 4 l.p.
9

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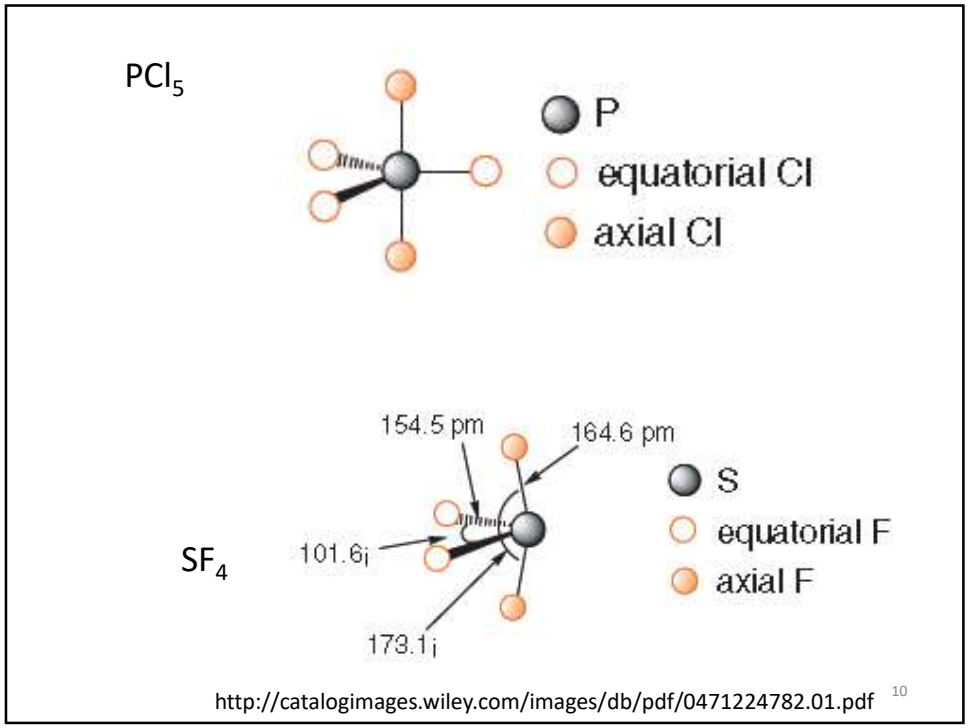
PCl5
P
equatorial Cl
axial Cl
154.5 pm
164.6 pm
101.6j
173.1j
SF4
S
equatorial F
axial F
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10

10

Magnitud de Repulsión de Pares Electrónicos

E – E >E - PE > PE- PE> E- Rad> PE- Rad > Rad-Rad

- E *Par libre*
- PE *Par Enlazado*
- Rad *Radical Libre*

11

11

Table 1.1 Shapes of molecules and ions

Number of central atom electron pairs	*Bonding pairs*	*Non-bonding pairs*	*Shape*	*Example*
2	2	0	Linear	$BeCl_2$
3	3	0	Triangular	BF_3
3	2	1	Bent	$SnCl_2$
4	4	0	Tetrahedral	CCl_4
4	3	1	Pyramidal	NH_3
4	2	2	Bent	H_2O
5	5	0	Trigonal bipyramidal (tbp)	PCl_5
5	4	1	Pseudo-tbp	SF_4
5	3	2	T-shaped	BrF_3
5	2	3	Linear	XeF_2
6	6	0	Octahedral	PF_6^-
6	5	1	Square pyramidal	IF_5
6	4	2	Square planar	IF_4^-

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12

Descripción General

AX_nE_m

- Donde ***A*** es el átomo central.
- ***X*** describe cualquier átomo alrededor de ***A.***
- ***E*** representa los pares de electrones libres *sobre el átomo central.*
- El *número de coordinación*, número de posiciones ocupadas por átomo o pares electrónicos alrededor de ***A***

13

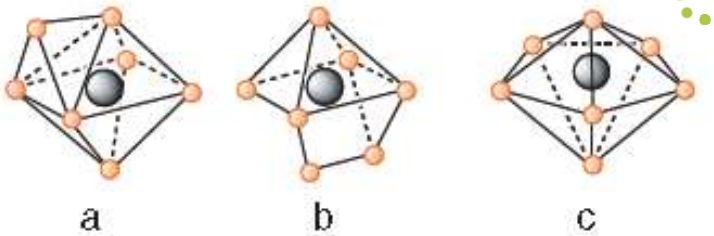
13

Molecules and Ions with Seven or More Electron Pairs

FAILS FOR:

Isoelectronic species

Transition metal compounds



Central atom

Points on a sphere, maximizing distance between them

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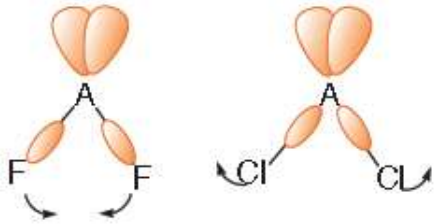
14

Atom Electronegativities

In an A–X bond between atoms A and X, as the atom X becomes more electronegative, the bonding pair occupies less space in the valence shell of atom A. In practice, this means that in a related series of compounds, bond angles of the type F–A–F are typically smaller than Cl–A–Cl or Br–A–Br angles



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15

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16

16