3. VSEPR Model
   Valence Shell Electron Pair Repulsion Theory

   Electron pairs will tend to stay as far apart as possible to minimize repulsions

   1.) Bonding Pairs B
   2.) Lone Pairs E
   3.) Central Atom A

   For $A\ B_x\ E_y$ which is the general notation

   X= # of B pairs   y = #of Lone Pairs

4. Occupancy factor = x + y
   Total number of electron pairs

Repulsions increase in the order:

Bonding Pair – Bonding Pair
Bonding Pair – Lone Pair
Lone Pair – Lone Pair

Q. Why?

A. Bonding Pair electrons are diffused through orbitals of A-B

AB_xE_y :

x+y	Basic Geometry	Hybridization
2	Linear	sp
3	Triangular	sp^2
4	Tetrahedral	sp^3, sd^3
	Square planar	dsp^2
5	Square pyramidal	dsp^3
	Trigonal bypyramidal	dsp^3
6	octahedral	d^2sp^3

Prototype Shapes for $AB_x E_y$

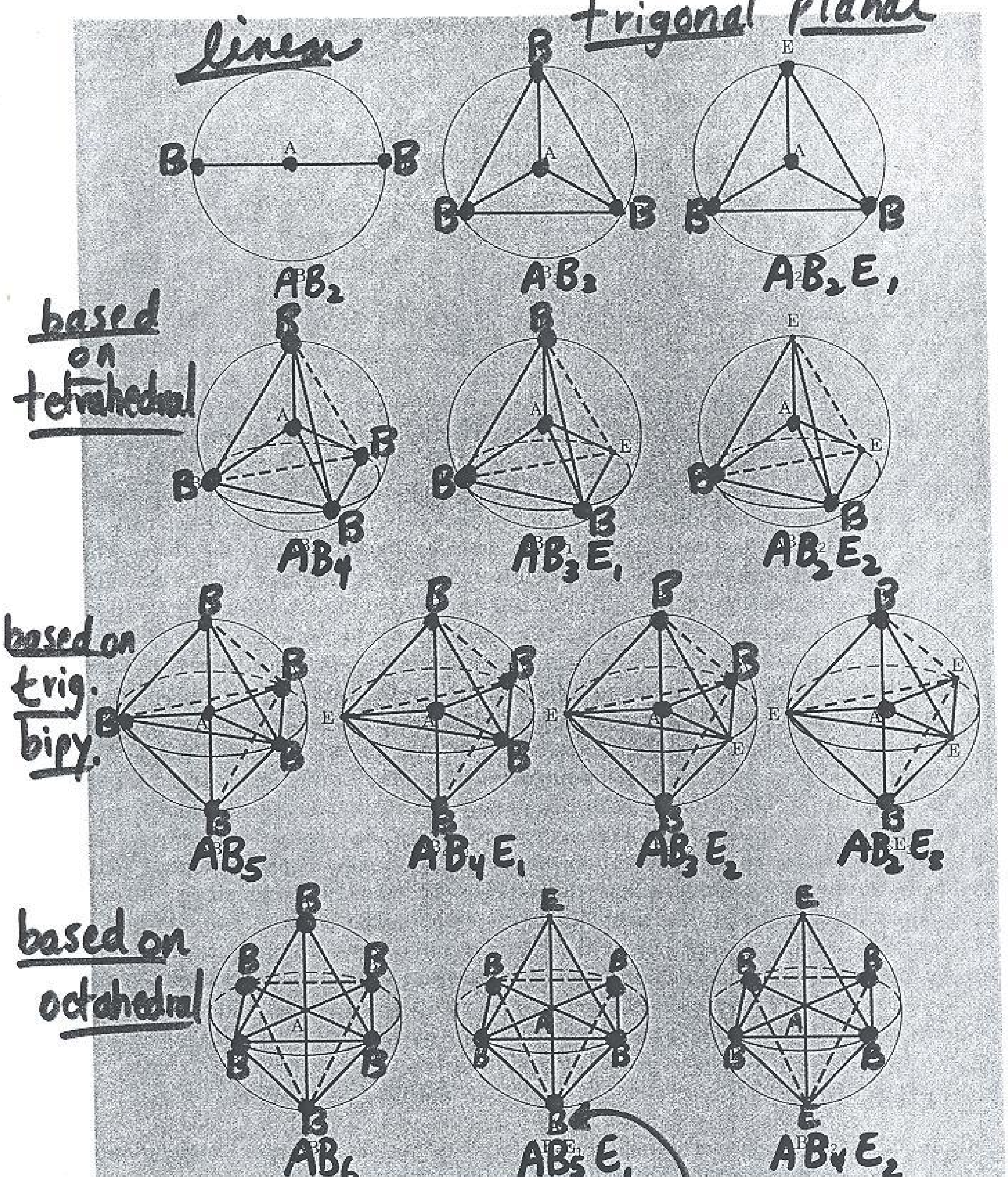


Figure 3-7 Idealized geometries for structures having the formulas AB_xE_y, where A is a central atom, B are peripheral atoms, and E are lone pairs residing on A.

mistake in the book it says 'A'

scription of the multiple bonds, and VSEPR adjustments of the prototype geometries.

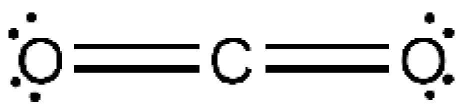
For every basic geometry type, there are different ways to achieve same occupancy factor x + y in the AB_xE_y formulae

occupancy of 2:

AB_2

x = 2
y = 0

linear



sp hybridized C
$\angle$ O-C-O = 180°

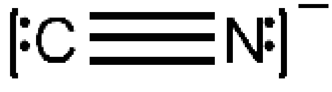
sp hybridized N
$\angle$ N-N-N = 180°

ABE

x = 1
y = 1

linear

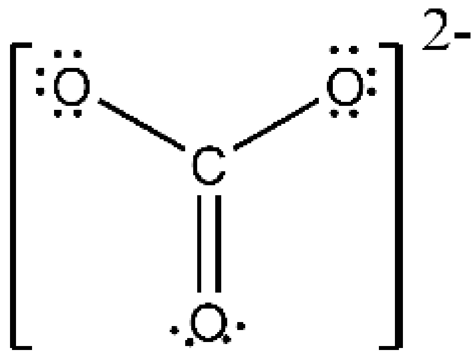
sp C, O



sp C, N

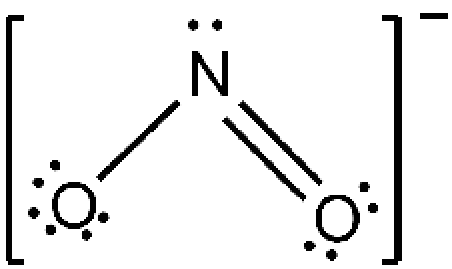
occupancy of 3:

AB_3
x = 3
y = 0
trigonal planar



sp^2 hybridized C
$\angle$O-C-O = 120°

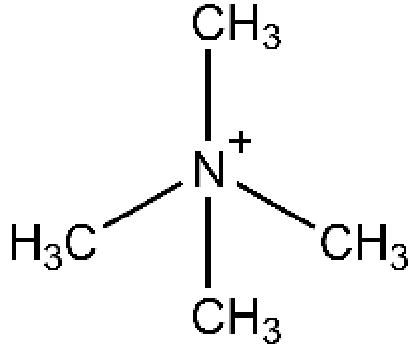
AB_2E
x = 2
y =1
bent



sp^2 hybridized N
$\angle$ O-N-O = 115°

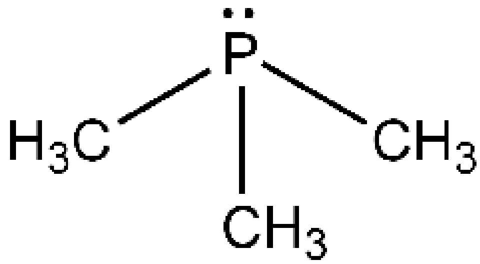
occupancy of 4:

AB_4
x = 4
y = 0
tetrahedral



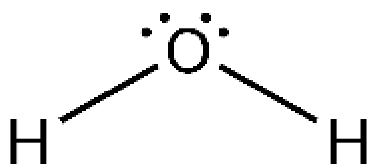
sp^3 hybridized N
$\angle$ C-N-C = 109°

AB_3E
x = 3
y = 1
<u>trigonal pyramid</u>



sp^3 hybridized P
∠ C-P-C = 99°

AB_2E_2
x = 2
y = 2
<u>bent</u>



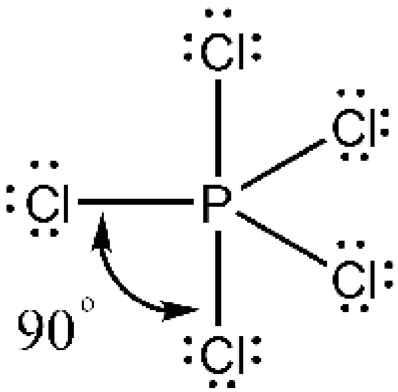
sp^3 hybridized O
∠ H-O-H = 104°

ABE_3
x = 1
y = 3
<u>linear</u>

presumably, sp^3 hybridized O, although with lone pairs it is hard to know where they really are in space!

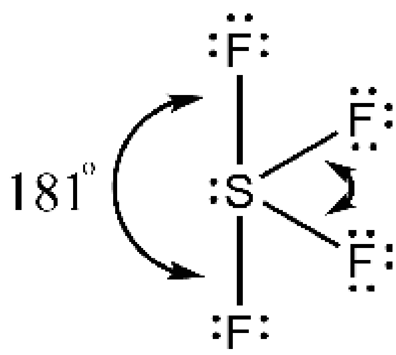
occupancy of 5:

AB_5
x = 5
y = 0
trigonal bipyramid (tbp)*



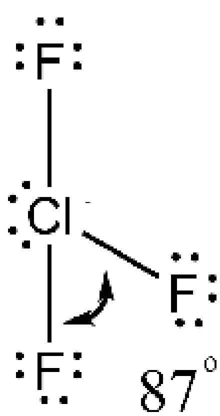
dsp^3 hybridized P
$\angle$ Cl-P-Cl = 120°
in $\triangle$ plane

AB_4E
x = 4
y = 1
saw-horse



dsp^3 hybridized S
$\angle$ F-S-F = 103°

AB_3E_2
x = 3
y = 2
T-shaped

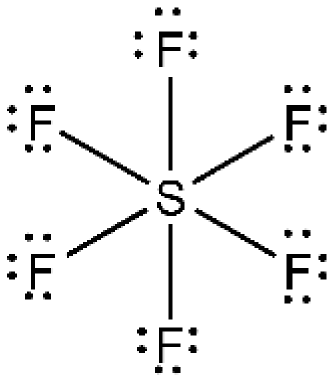


dsp^3 hybridized Cl

*note that tbp is the most common AB_5 basic geometry

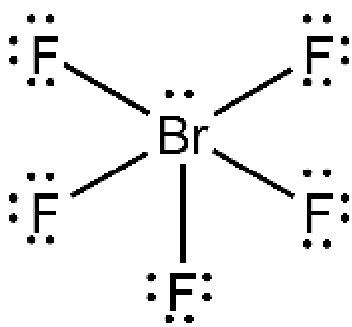
occupancy of 6:

AB_6
x = 6
y = 0
octahedron



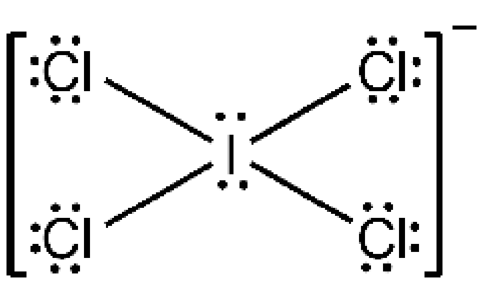
d^2sp^3 hybridized S

AB_5E
x = 5
y = 1
square pyramid



d^2sp^3 hybridized Br

AB_4E_2
x = 4
y = 2
square planar



d^2sp^3 hybridized I

Summary of main types of Hybridization & shapes of orbitals

1) sp – linear
2) sp^2 – trigonal planar
3) sp^3 — tetrahedral
4) sd^3 — tetrahedral
5) dsp^2
6) dsp^3
   a) $d_{z^2}sp^3$ → trigonal bipyramidal
   b) $d_{x^2-y^2}sp^3$ → square pyramid
7) d^2sp^3 octahedral

Occupancies for:

$sp = 2$	$dsp^2 = 4$
$sp^2 = 3$	$dsp^3 = 5$
$sp^3 = 4$	$d^2sp^3 = 6$
$sd^3 = 4$	

} Occupancy is how many orbitals you are using

Main Point:

Armed With:

1) An understanding of how to draw Lewis structures

2) How to determine occupancies of a molecule (bonding + lone pairs)

We can use (1) and (2) to predict structures by both the Hybridization and the VSEPR methods & correlate them

<u>Process of applying Lewis structures VSEPR and Hybridization:</u>

(1) Determine the Lewis Structure Diagram

(2) Determine occupancy factor x+y

(3) Determine how many hybrid orbitals you will need (same as x+y) and choose type of hybridization.
   a) use only s, p orbitals for elements in rows 1,2 (elements below Ne which is #10)
   b) s,p and d orbitals are all available after row 2
   c) note that multiple bonds can be made from unhybridized orbitals

(4) from the occupancy factor (x+y) determine a basic geometry type. After arranging the Bonding Pairs and Lone Pairs, determine the actual geometry of the molecule.

Example 1:

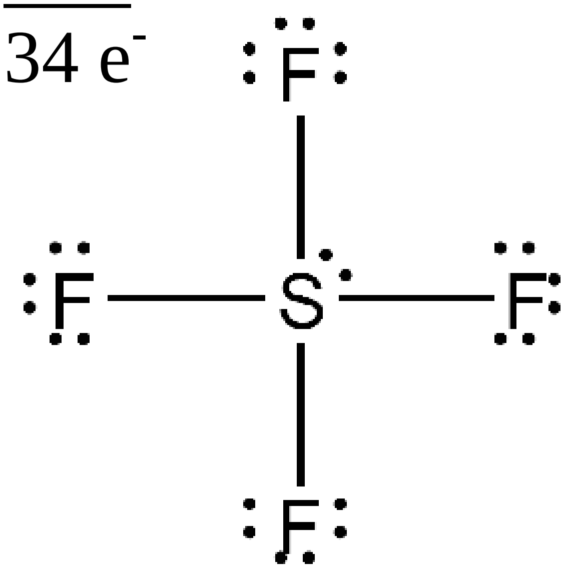
SF_4

(1) Lewis Structure

A: S $6\ e^-$ $6\ e^-$

B: F $7\ e^- \times 4 =$ $\underline{28\ e^-}$

$34\ e^-$



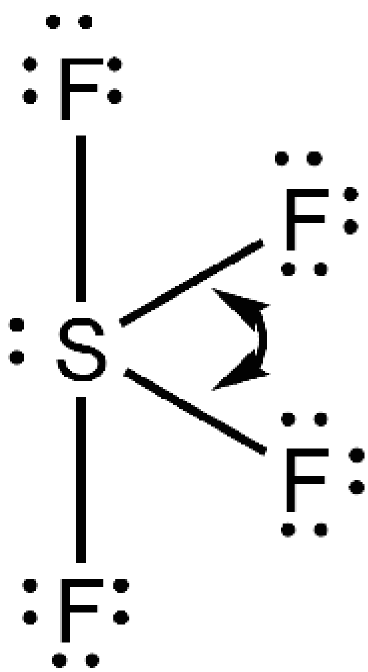
(2) AB_4E

occupancy = 5

(3) for an occupancy of 5, with d orbitals available we have dsp^3 hybridization.

(5) for an occupancy of 5, AB_4E, one can either a trigonal bipyramid or square pyramidal Tbp is, by far, the most common.

so tbp is the <u>Basic Geometry</u>, but saw-horse is actual structure with the atoms



angle is < 120°
because of l.p.-b.p.
repulsion being
greater than b.p.-b.p.