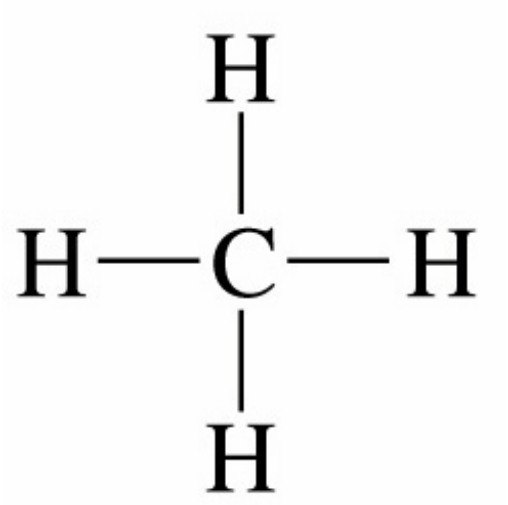
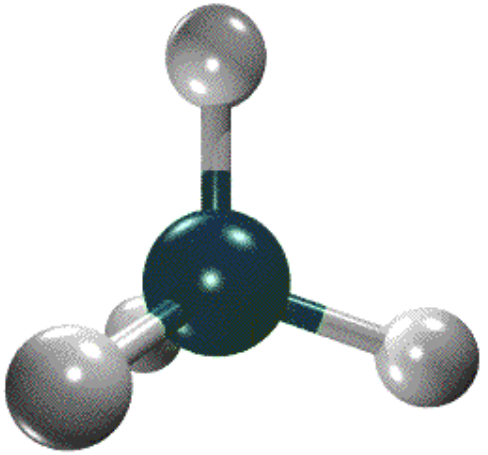
Chemical Bonding II: Molecular Geometry

Lewis structures do not show 3D shape of molecules





Molecular Geometry

Valence Shell Electron Pair Repulsion

A simple but effective model for predicting shape (geometry) of molecules

Molecular Geometry

Valence Shell Electron Pair Repulsion

A simple but effective model for predicting shape (geometry) of molecules

Molecular Geometry

VSEPR theory

* VSEPR *

The VSEPR theory assumes:

molecules adopt a shape that minimizes the repulsive force among a given number of electron pairs

molecules have a 3 D shape

VSEPR - must know Lewis structure

Number of atoms in molecule

Number of bonding & nonbonding electrons on central atom

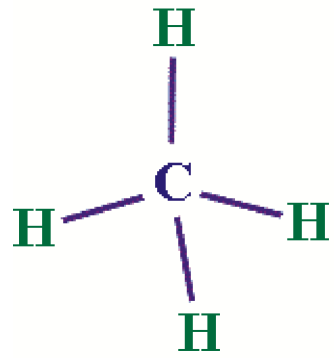
Names of shapes
How to draw shapes

Table 10.1

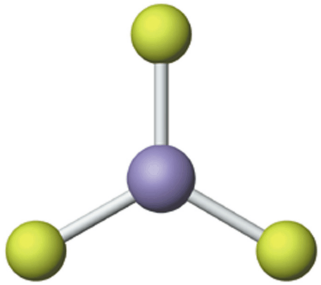
* VSEPR *

molecular shapes can be represented in several ways

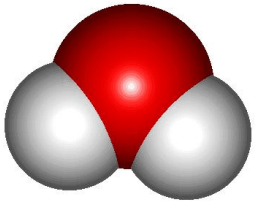
- **perspective drawing**



- **ball and stick model**



- **space filling model**



VSEPR Theory

Divide molecules into 2 classes

1. molecules in which the central atom has no nonbonding electrons

2. molecules in which the central atom has nonbonding electrons

VSEPR Theory

Divide molecules into 2 classes

1. molecules in which the central atom has no nonbonding electrons

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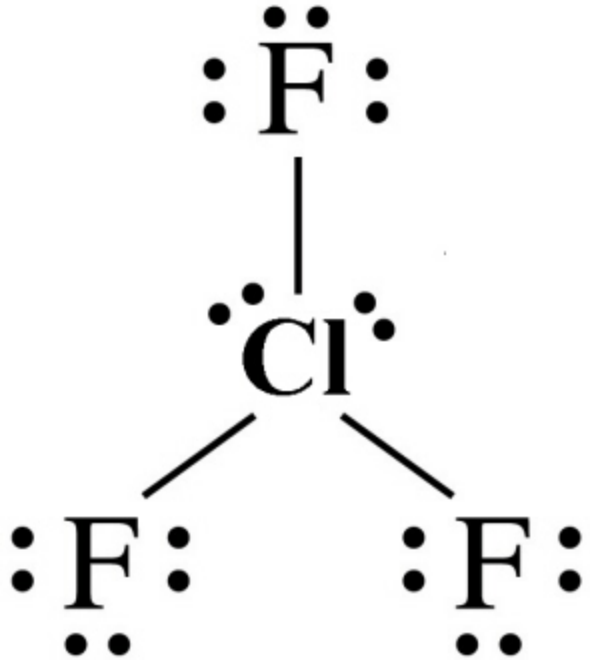
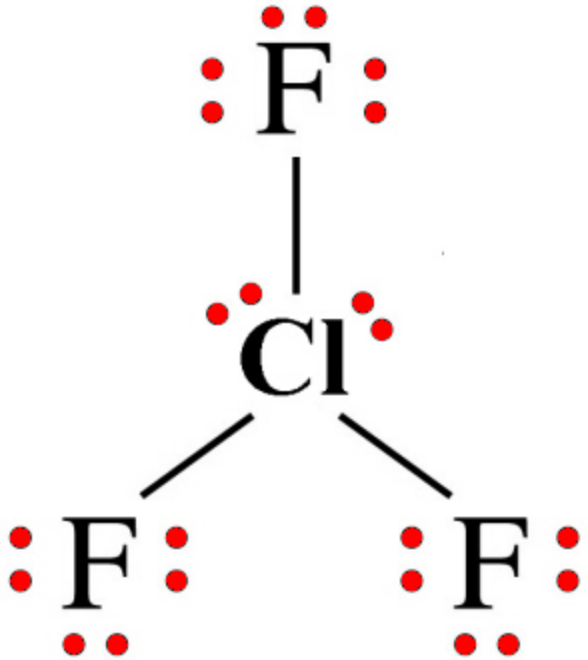
VSEPR Theory

compare bonding & nonbonding e^-



VSEPR Theory

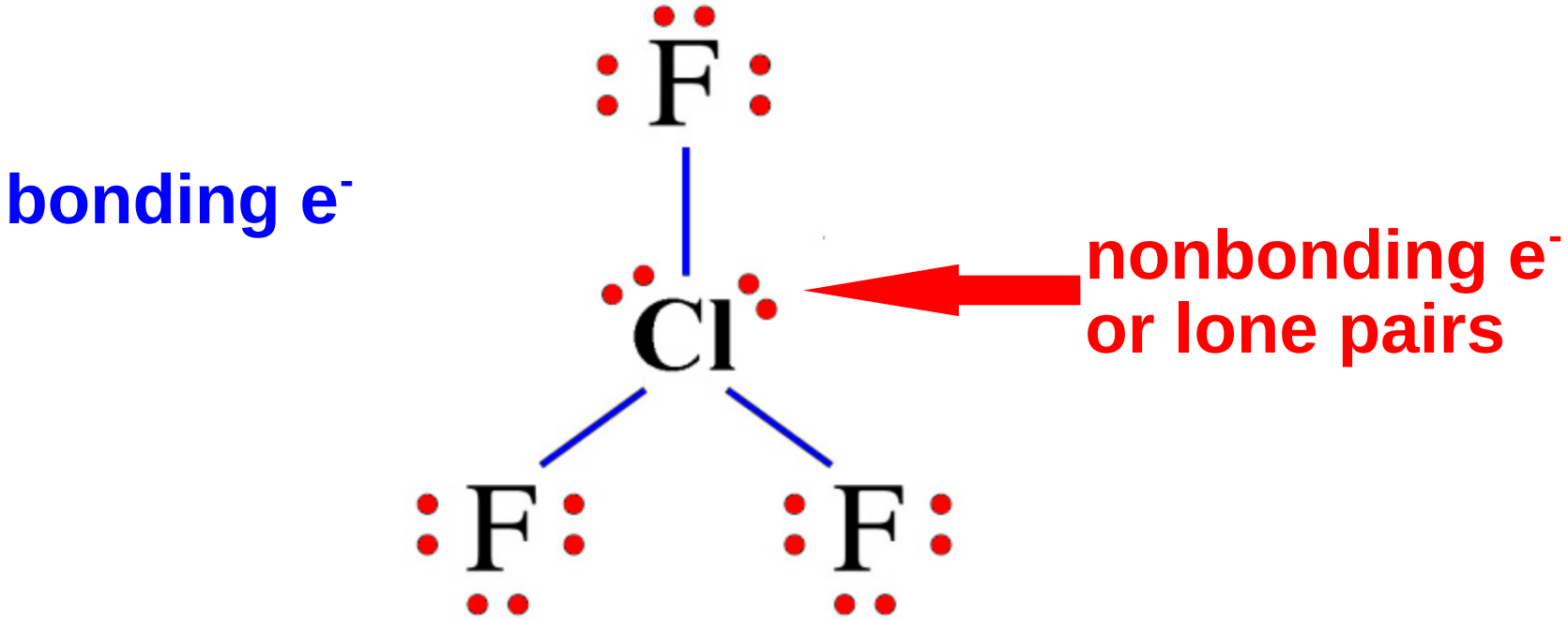
compare bonding & nonbonding e^-



nonbonding e^- or lone pairs

VSEPR Theory

compare bonding & nonbonding e^-



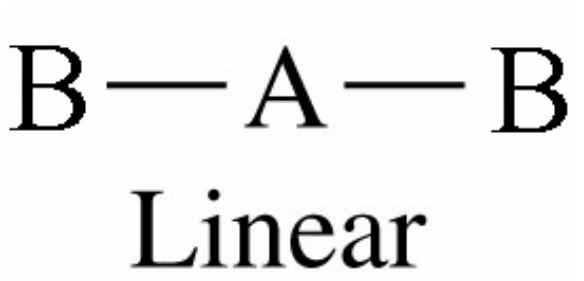
VSEPR Theory

simple AB_x molecules

A central atom
B terminal atoms
x = 2-6
x can be >6

VSEPR Theory

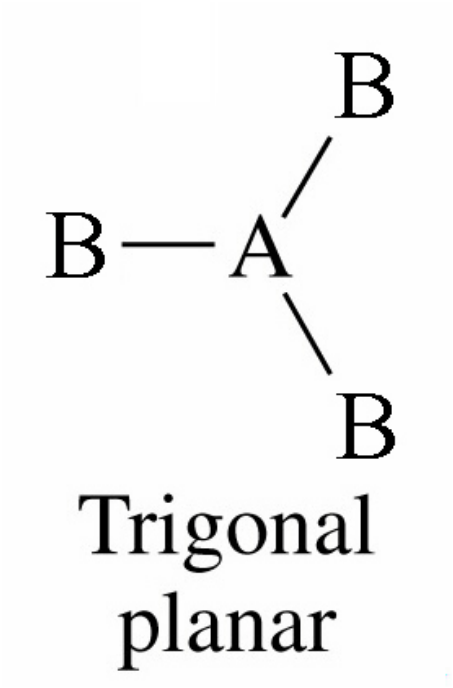
1. x = 2 ± AB_2



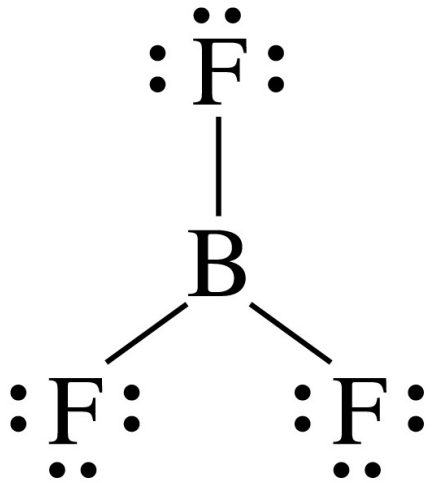
$BeCl_2$

VSEPR Theory

1. x = 3 ± AB_3

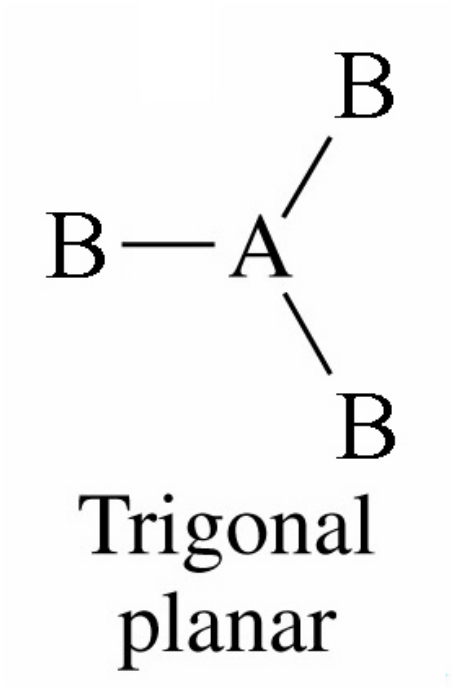


BF_3

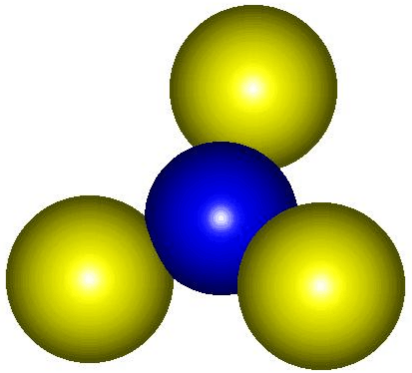


VSEPR Theory

1. x = 3 ± AB_3

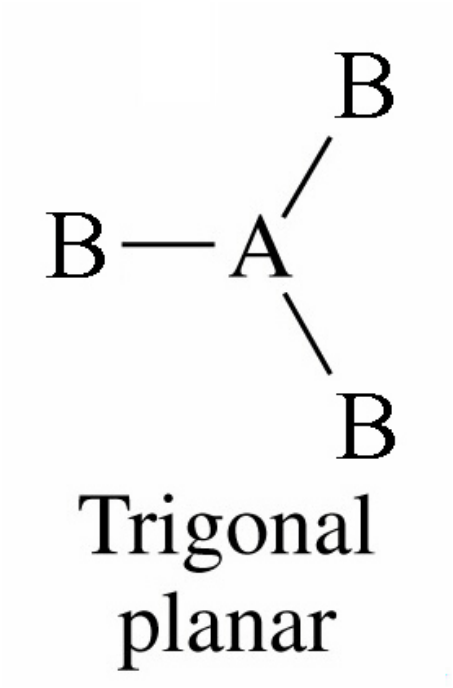


BF_3

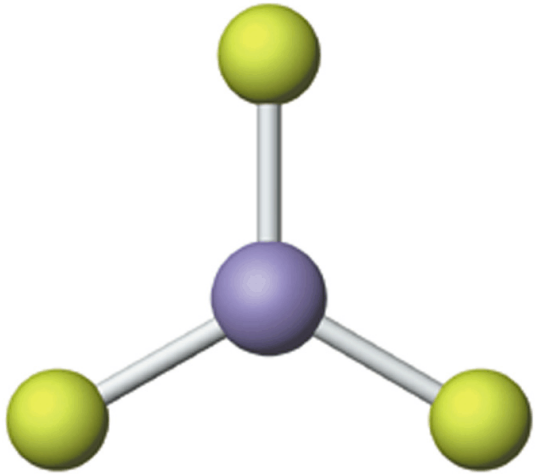


VSEPR Theory

1. x = 3 ± AB_3

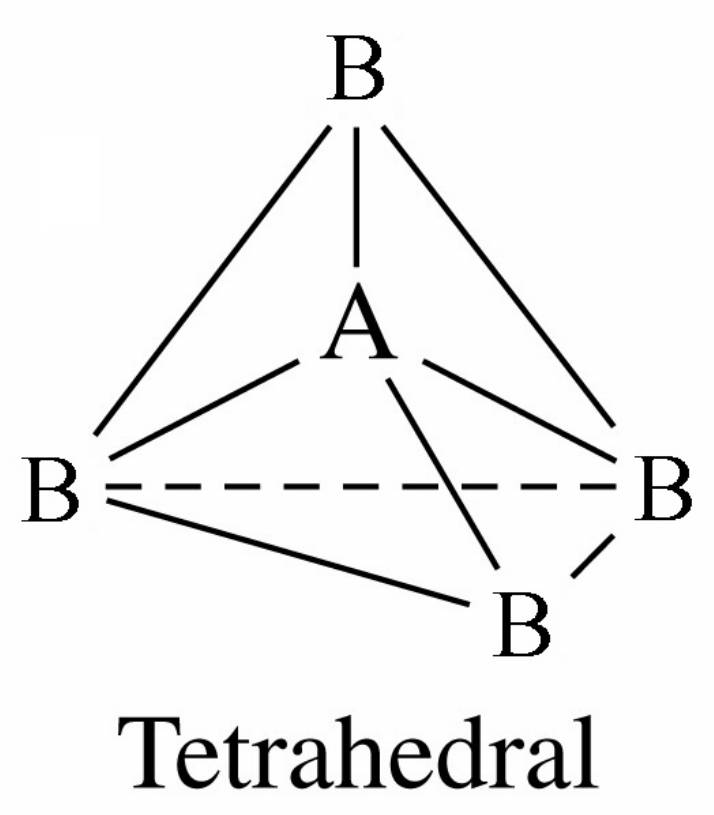


BF_3

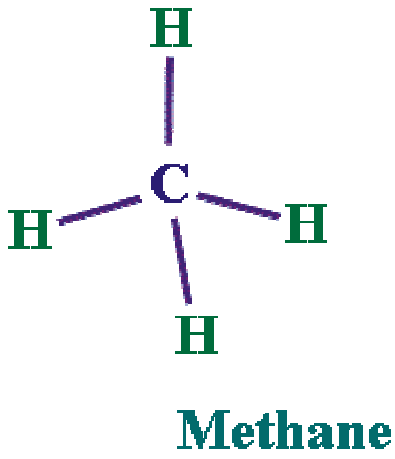


VSEPR Theory

1. x = 4 ± AB_4

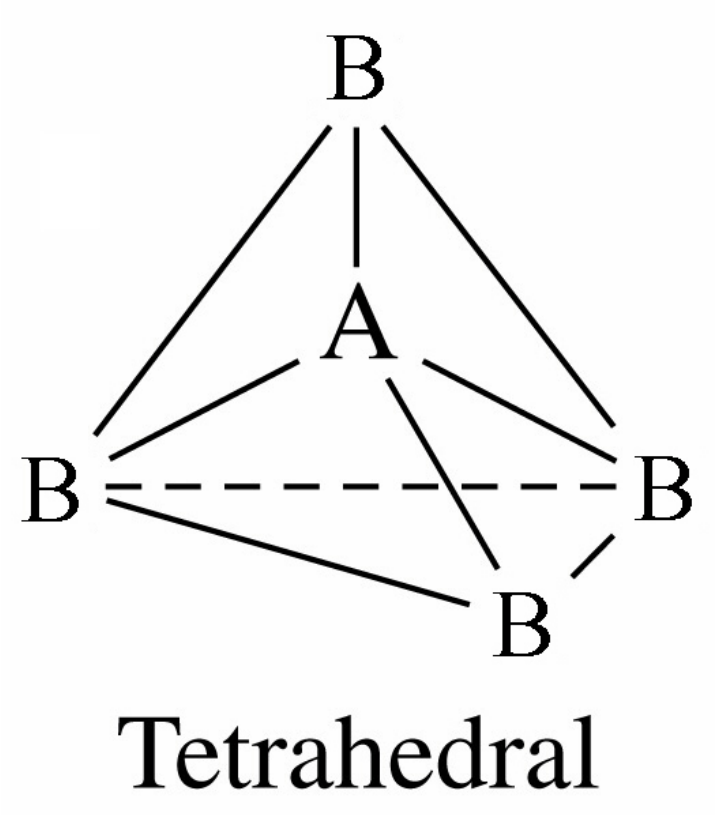


CH_4

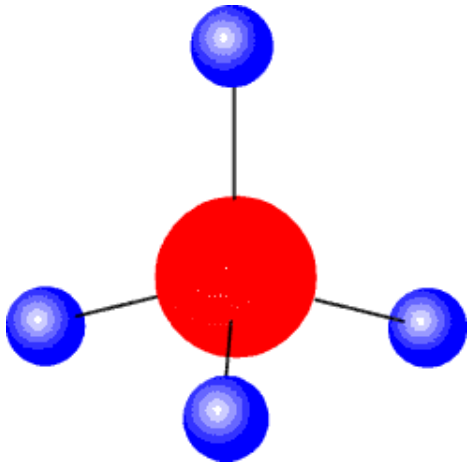


VSEPR Theory

1. x = 4 ± AB_4



CH_4



VSEPR Theory

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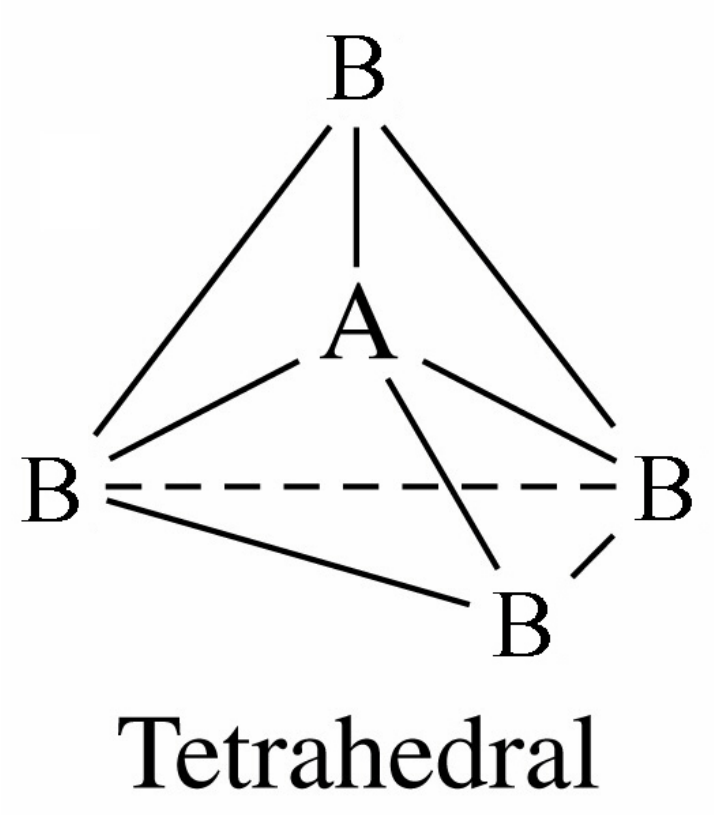
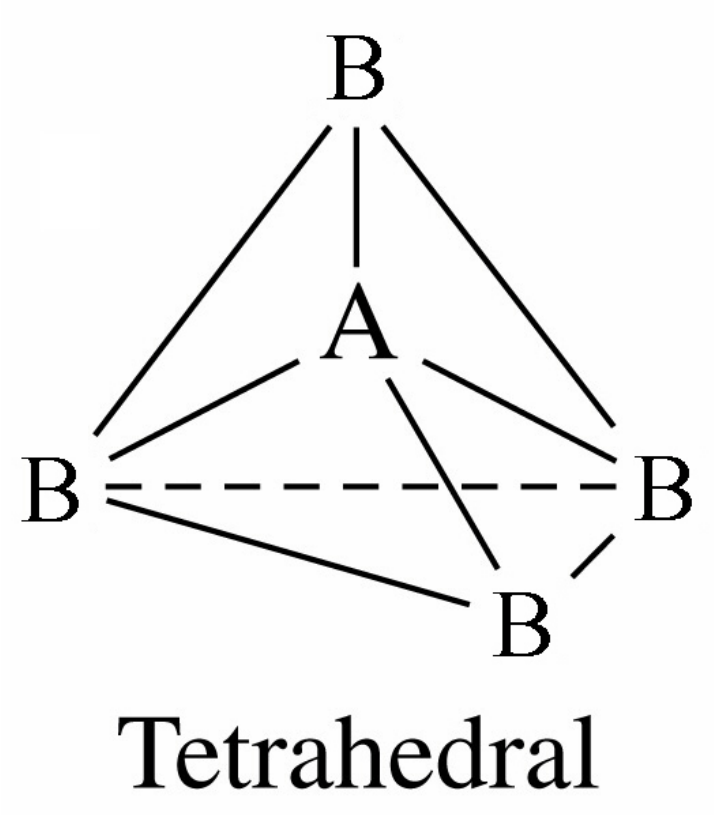


CH_4

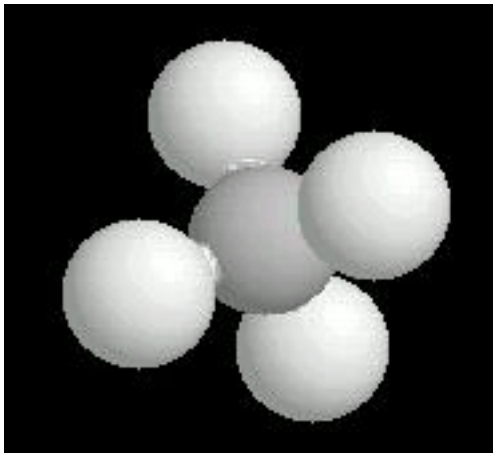
C H

VSEPR Theory

1. x = 4 ± AB_4



CH_4



VSEPR Theory

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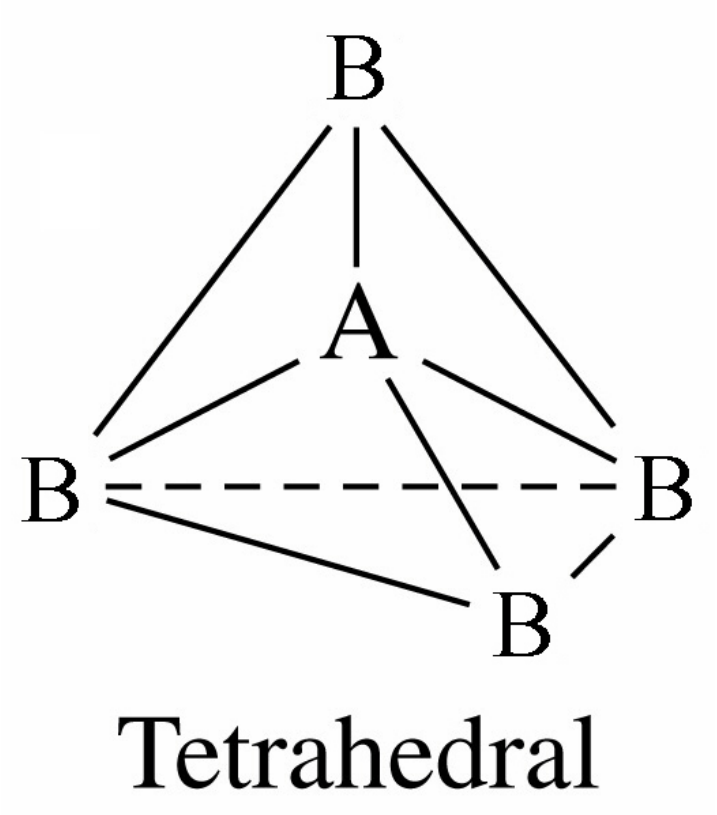
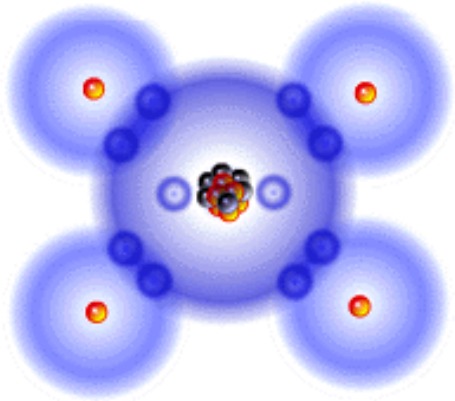


CH_4



VSEPR Theory

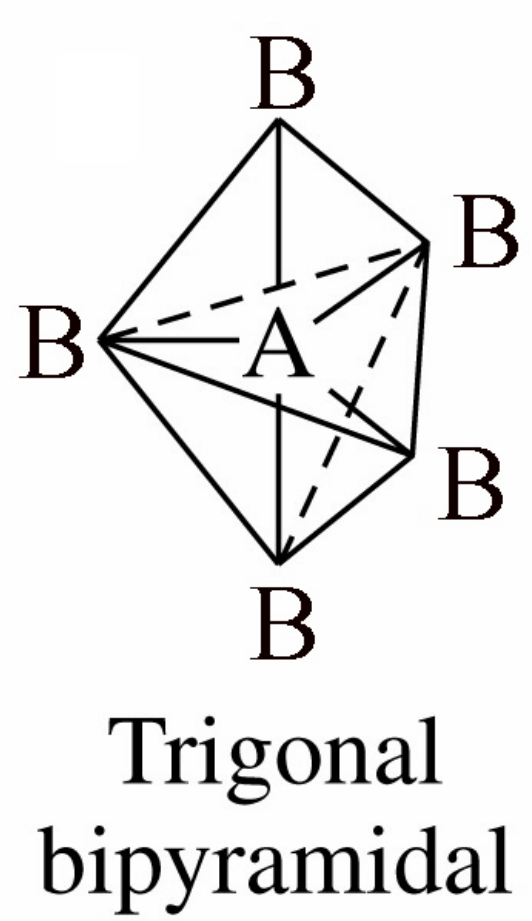
Properties:

- **flammable**
- **produced by bacteria in gut of mammals**

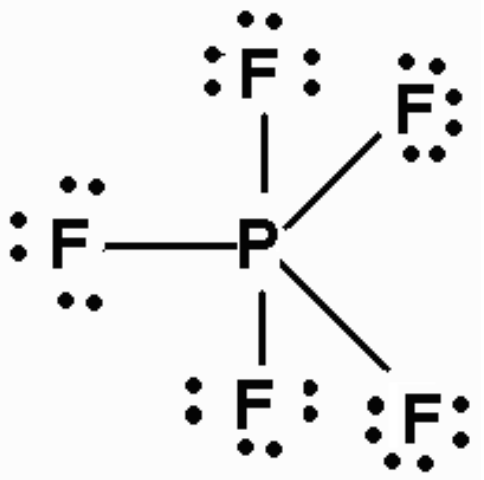
CH_4

VSEPR Theory

1. x = 5 ± AB_5

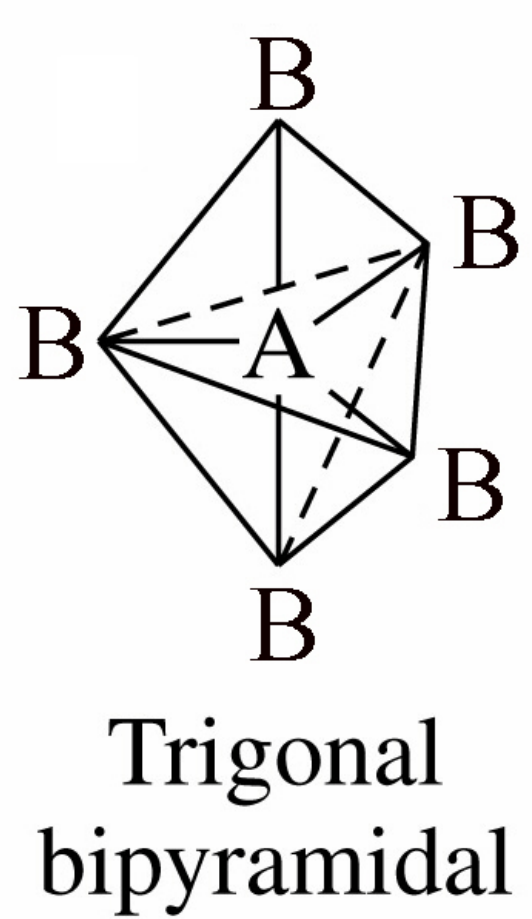


PF_5



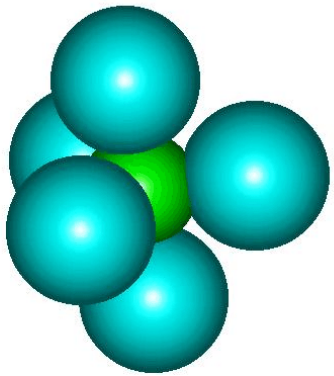
VSEPR Theory

1. x = 5 ± AB_5



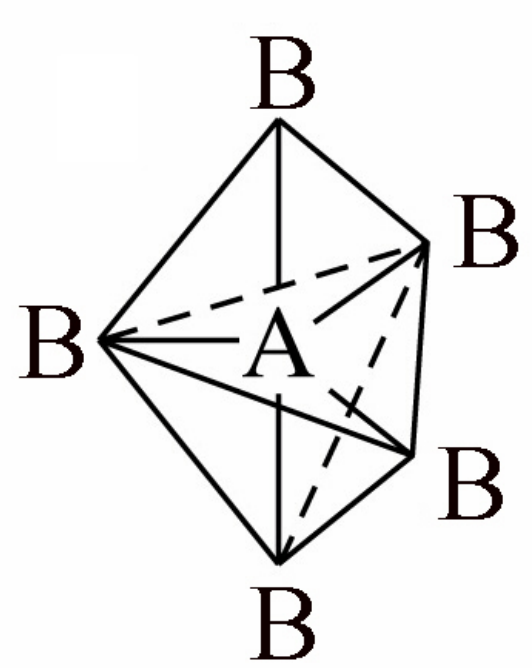
Trigonal bipyramidal

PF_5



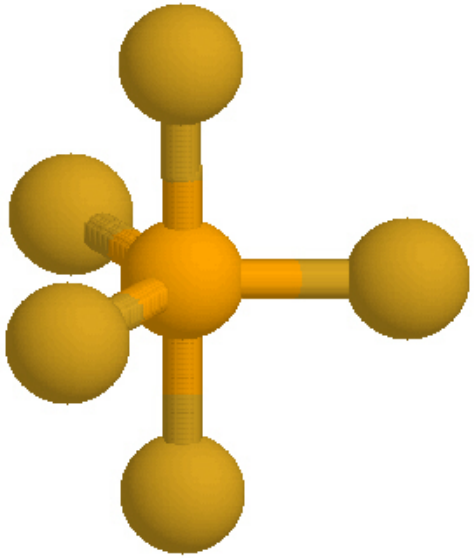
VSEPR Theory

1. x = 5 ± AB_5



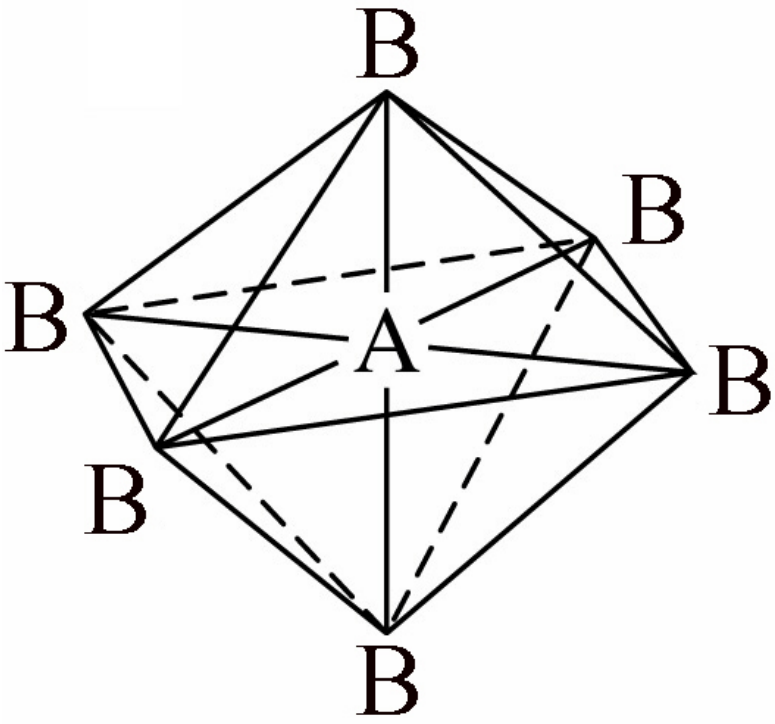
Trigonal bipyramidal

PF_5

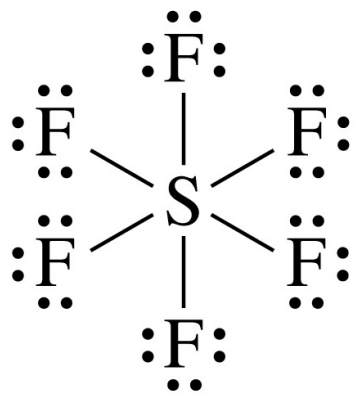


VSEPR Theory

1. x = 6 ± AB_6



Octahedral

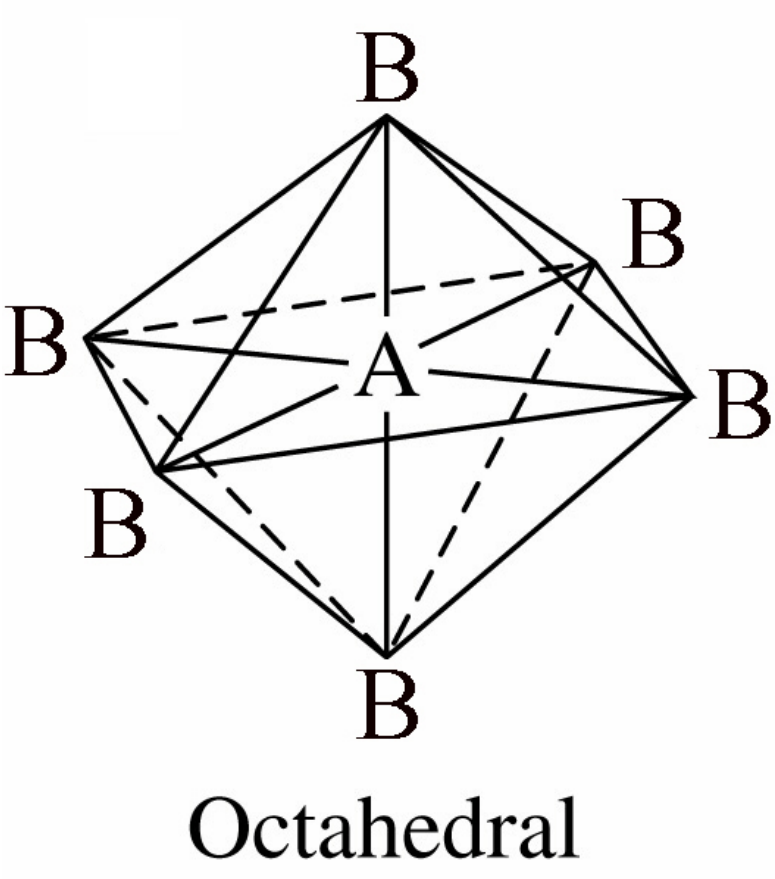


Sulfur hexafluoride

SF_6

VSEPR Theory

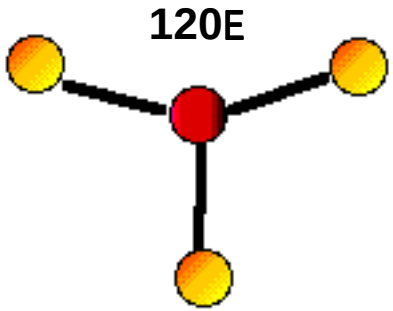
1. x = 6 ± AB_6



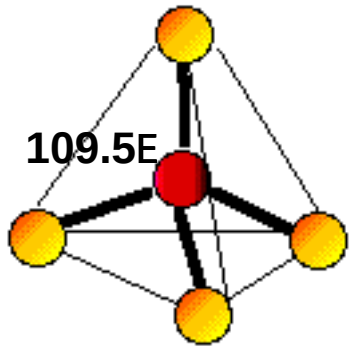
SF_6

Bond Angles

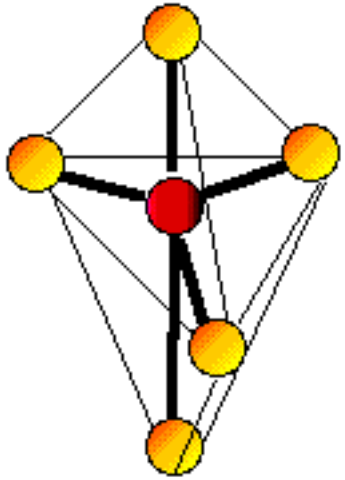
LINEAR



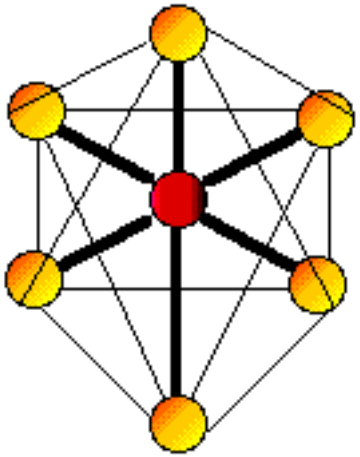
TRIGONAL PLANAR



TETRAHEDRAL



TRIGONAL BIPYRAMIDAL



OCTAHEDRAL

VSEPR Theory

Divide molecules into 2 classes

1. molecules in which the central atom has no nonbonding electrons

2. molecules in which the central atom has nonbonding electrons

VSEPR Theory

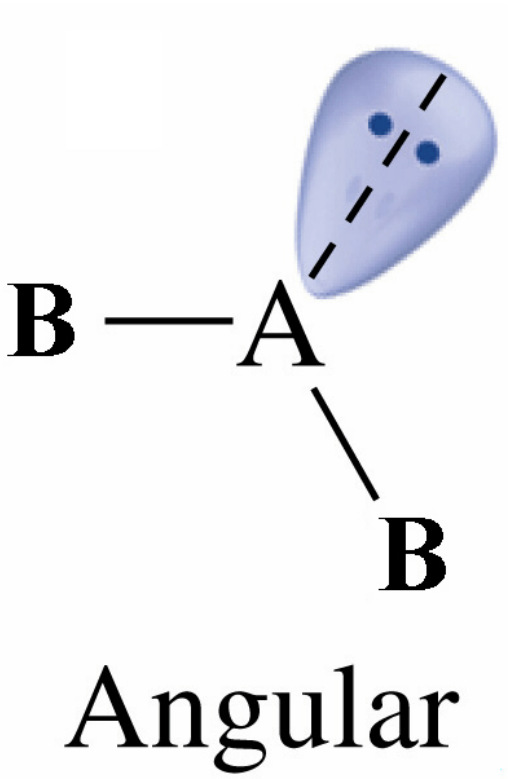
general formula ± AB_xE_y

A central atom
B terminal atoms
E lone pairs
x = 2-5
y = 1-3

Table 10.2

VSEPR Theory

1. x = 2; y = 1 ± AB_2E



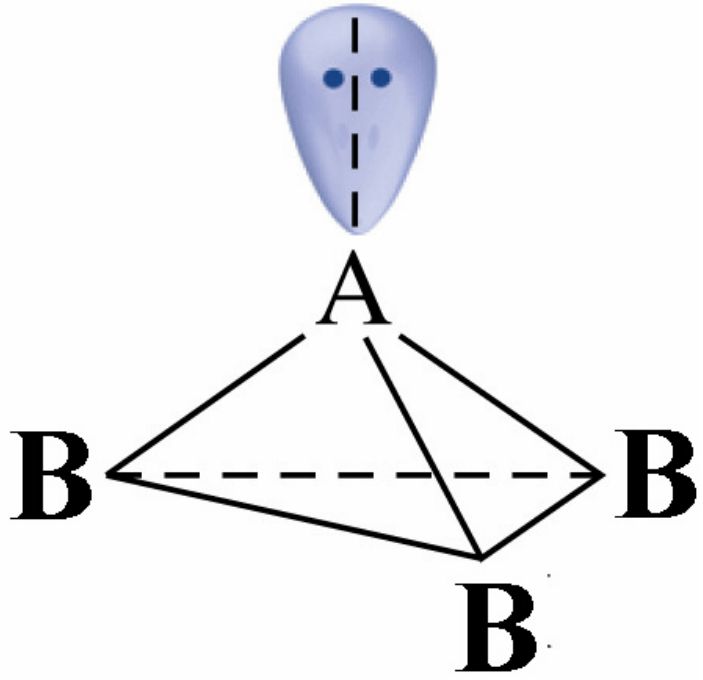
SO_2

Angular

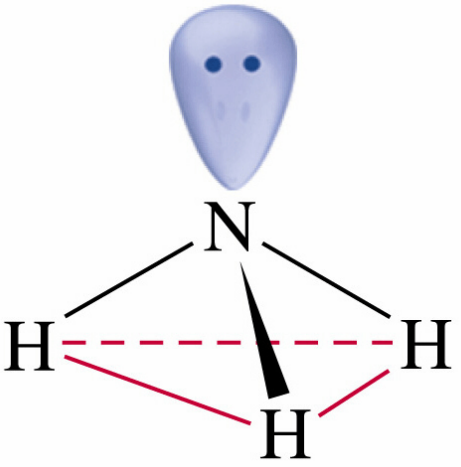
VSEPR Theory

2. x = 3; y = 1 ± AB_3E

NH_3

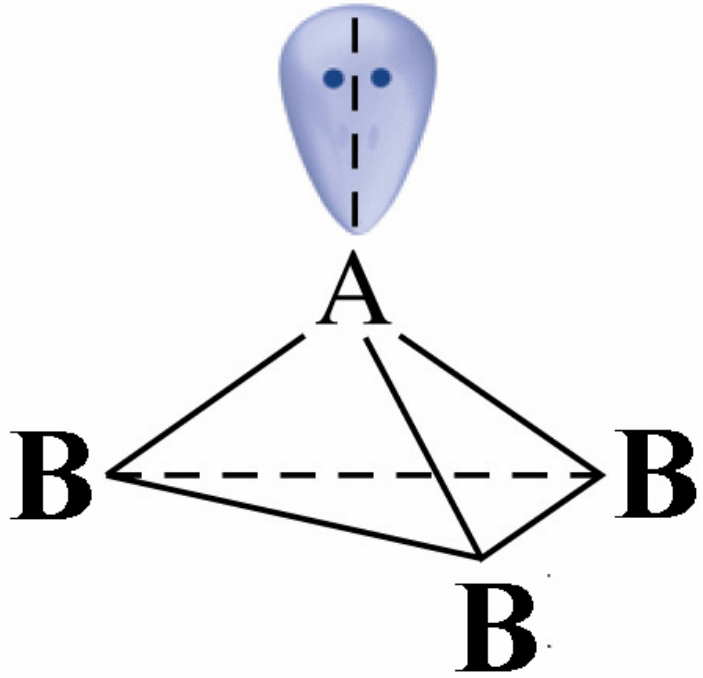


Trigonal pyramidal



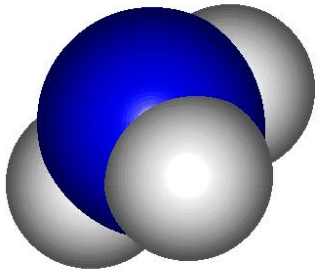
VSEPR Theory

2. x = 3; y = 1 ± AB_3E



Trigonal pyramidal

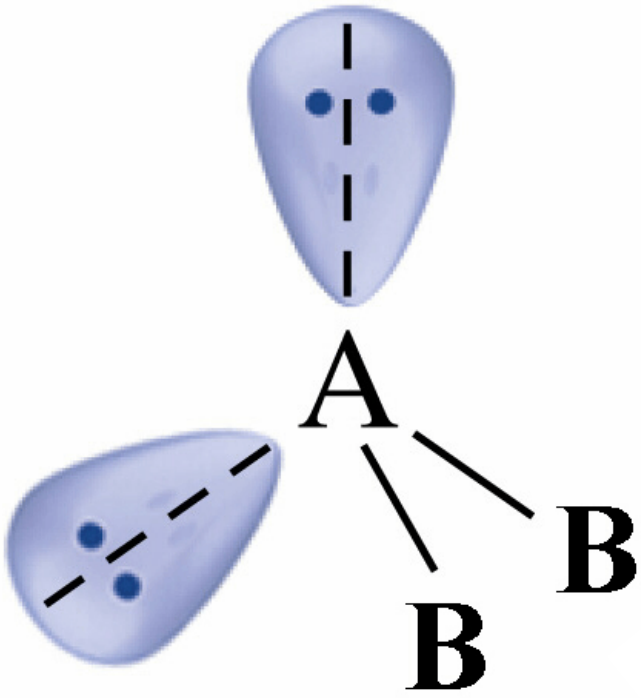
NH_3



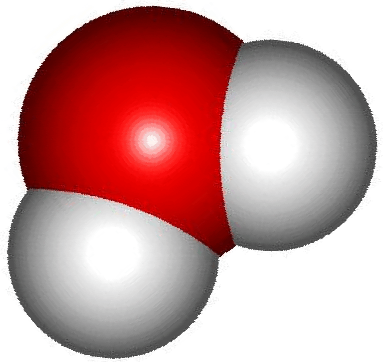
VSEPR Theory

3. x = 2; y = 2 ± AB_2E_2

H_2O



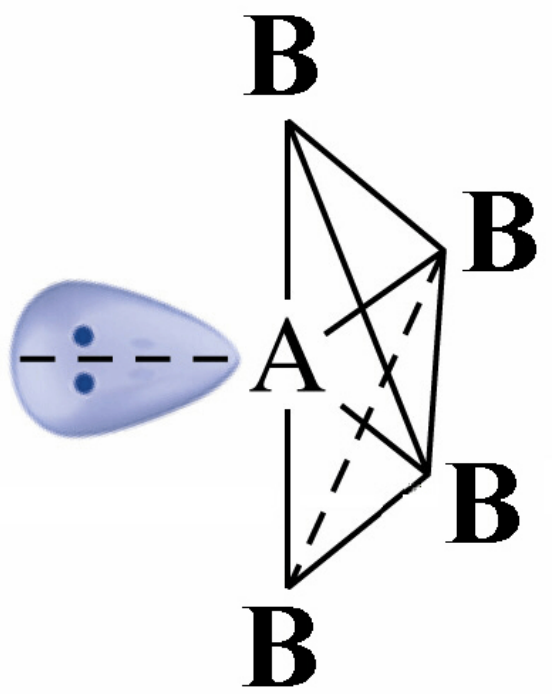
Angular



VSEPR Theory

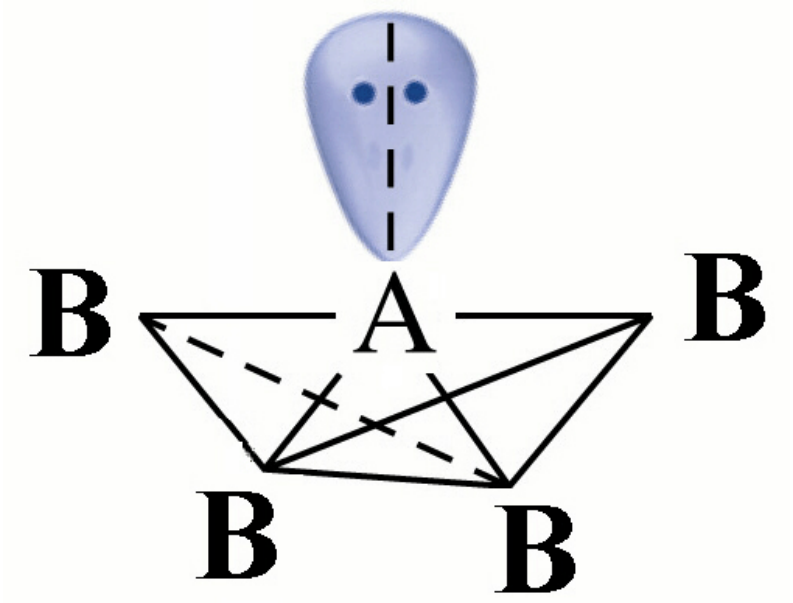
4. x = 4; y = 1 ± AB_4E

SF_4



VSEPR Theory

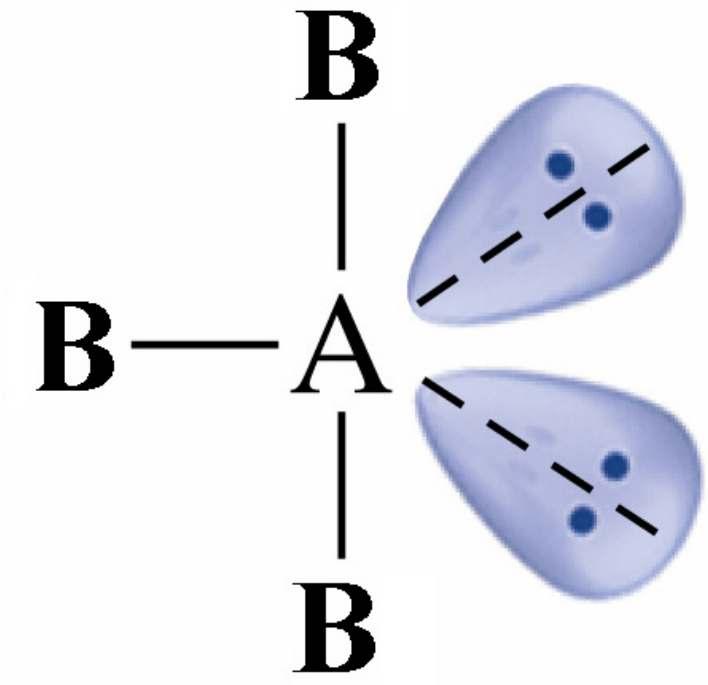
4. x = 4; y = 1 ± AB_4E



SF_4

VSEPR Theory

5. x = 3; y = 2 ± AB_3E_2



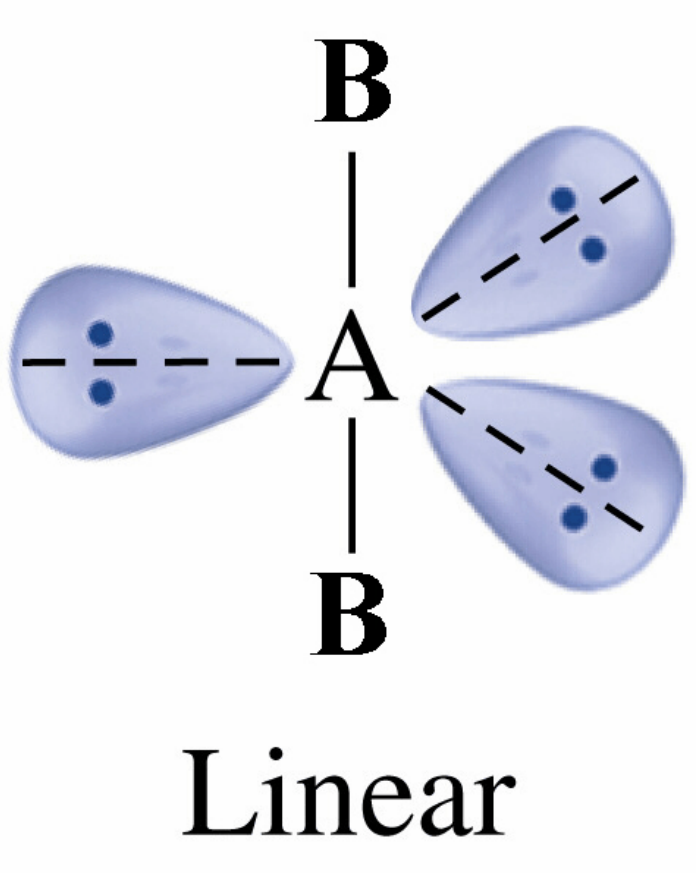
ClF_3

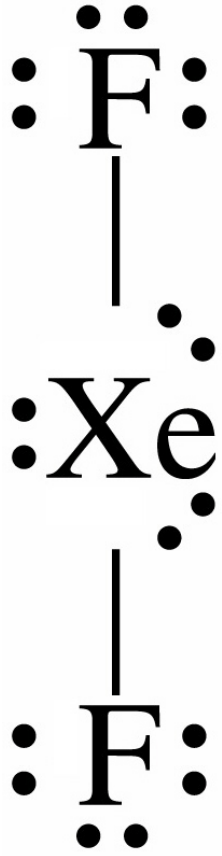
T-shaped

VSEPR Theory

6. x = 2; y = 3 ± AB_2E_3

XeF_2

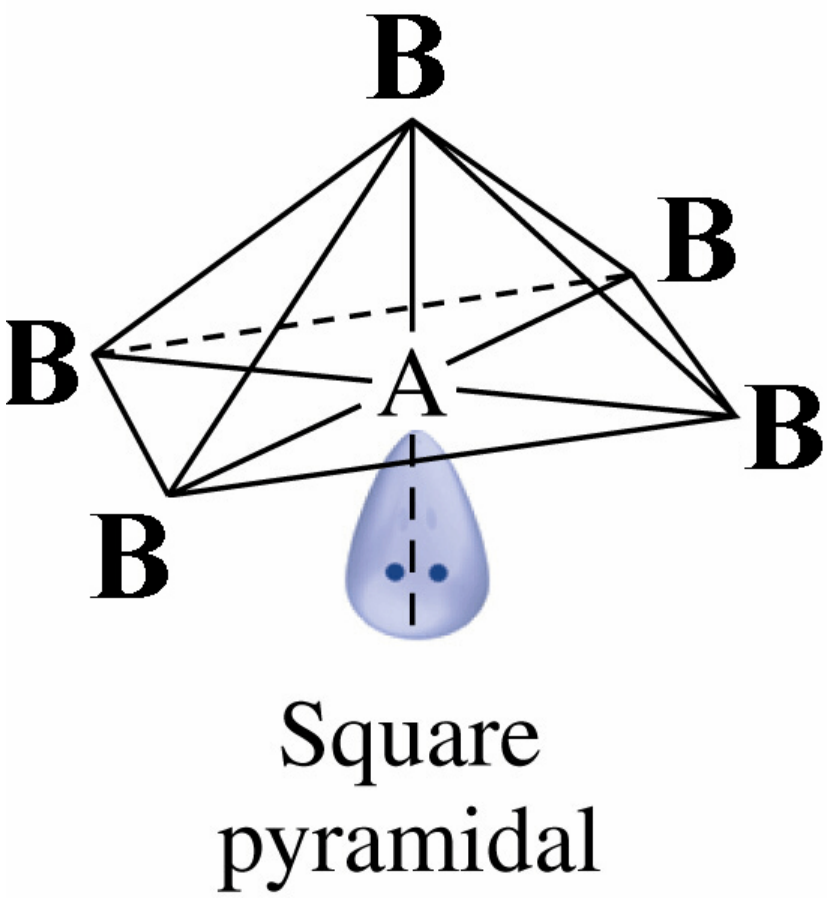




VSEPR Theory

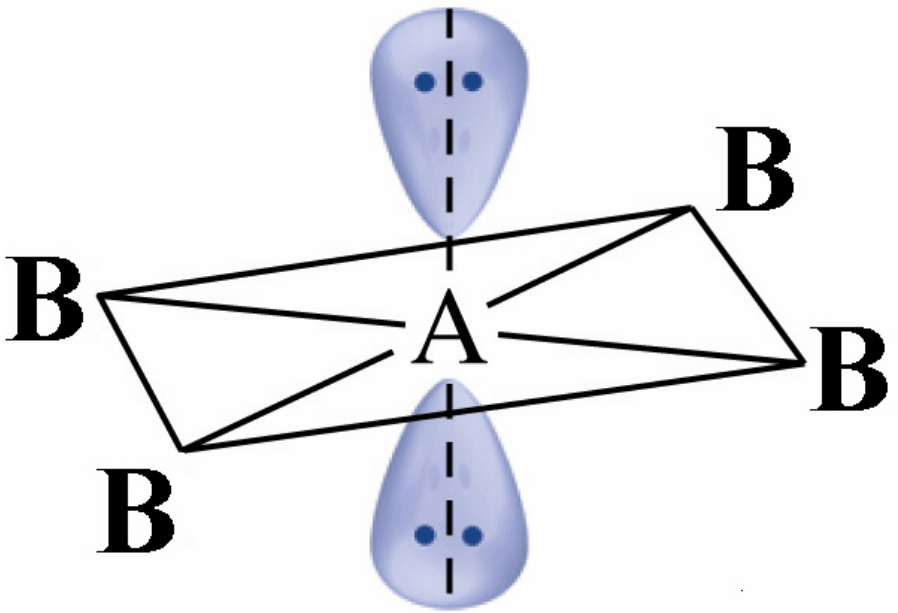
7. x = 5; y = 1 ± AB_5E_1

BrF_5



VSEPR Theory

8. x = 4; y = 2 ± AB_4E_2



XeF_4

Square planar

VSEPR Theory

How to determine geometry from a chemical formula ?

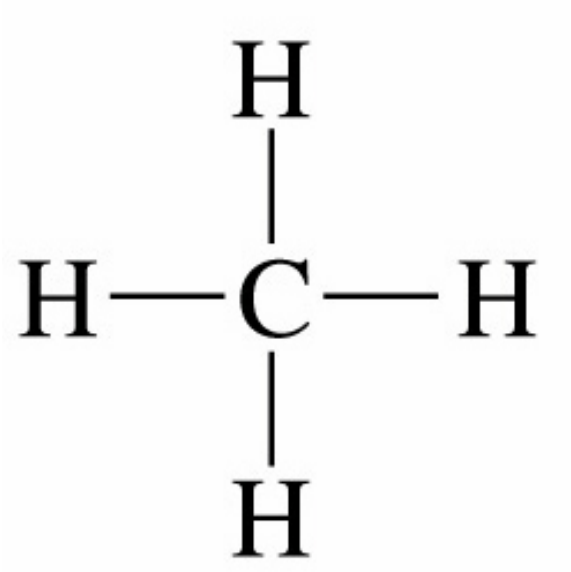
Draw & name geometry of CH_4

VSEPR Theory

1. **Write Lewis structure**
2. **Find number of bonding & nonbonding e^- on central atom**
3. **Determine correct shape from Tables 10.1 & 10.2**

VSEPR Theory

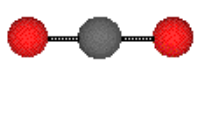
Draw & name geometry of CH_4



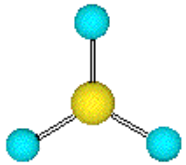
4 bonding pairs
0 nonbonding pairs

AB_4

go to tables

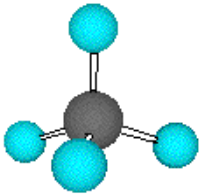


AX_2 Linear

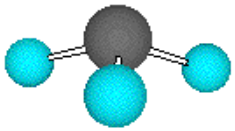


AX_3 Trigonal Planar

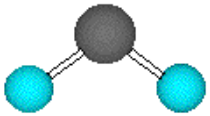
AX_2E Bent



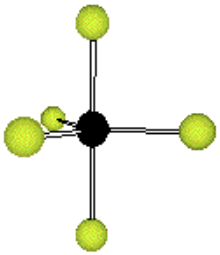
AX_4 Tetrahedral



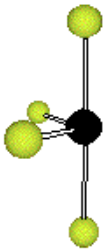
AX_3E Pyramidal



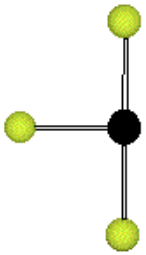
AX_2E_2 Bent



AX_5 Trigonal Bipyrimadal

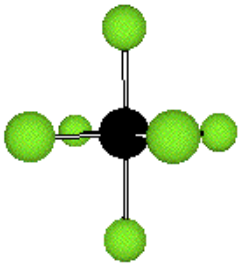


AX_4E Seesaw

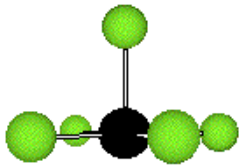


AX_3E_2 T-shaped

AX_2E_3 Linear



AX_6 Octahedral

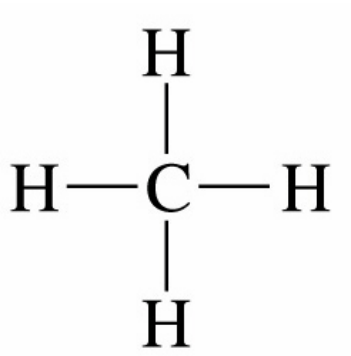


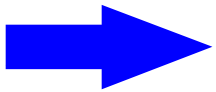
AX_5E Square Pyramidal

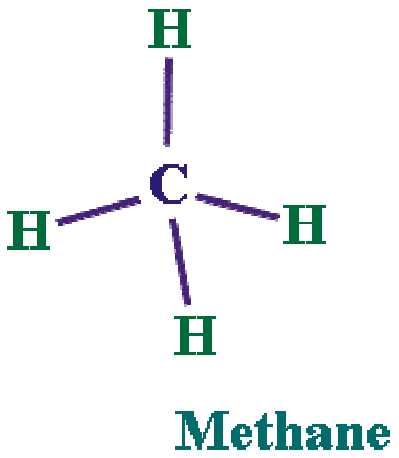
AX_4E_2 Square Planar

VSEPR Theory

Draw & name geometry of CH_4





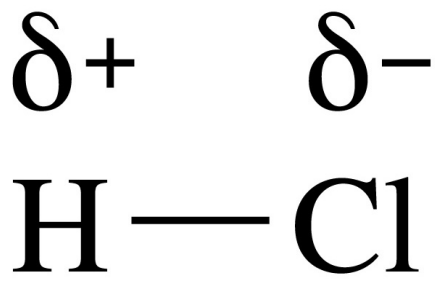


tetrahedral

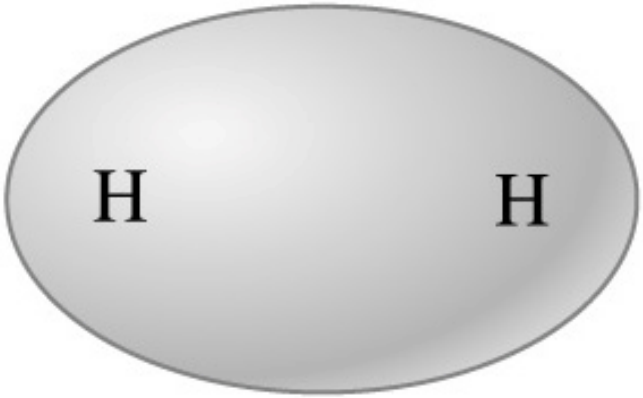
Dipole Moments

Physical property symbol :
units debye (D)

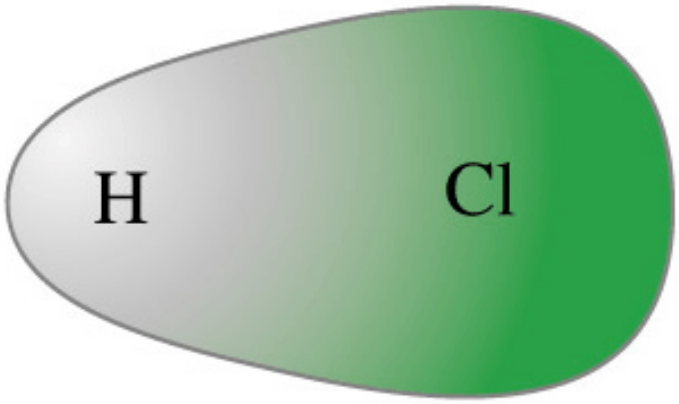
measures extent of polarity



Nonpolar covalent bond



Polar covalent bond



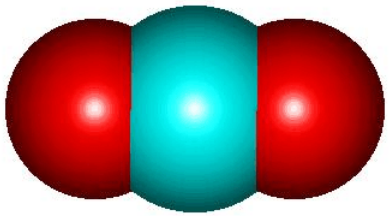
Dipole Moments

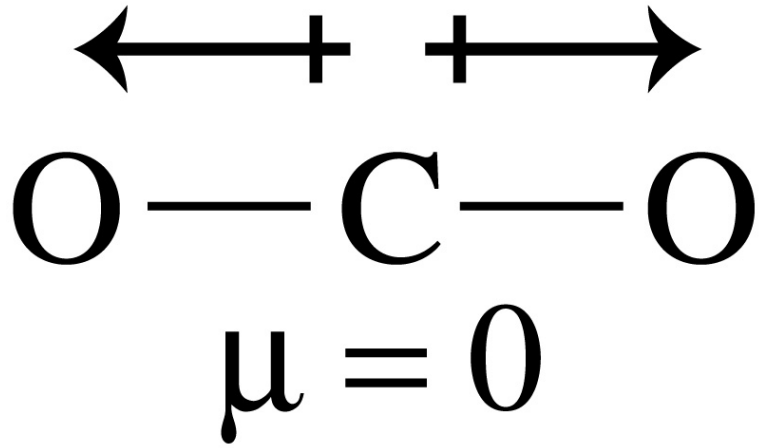
bond	:
H-H:	0
H-F:	1.92
H-Cl:	1.08
H-Br:	0.78

$$\overset{\delta+}{H}—\overset{\delta-}{Cl}$$

Dipole Moments

For molecules with > 1 bond:
dipole is vector sum
may or may not = 0





Dipole Moments

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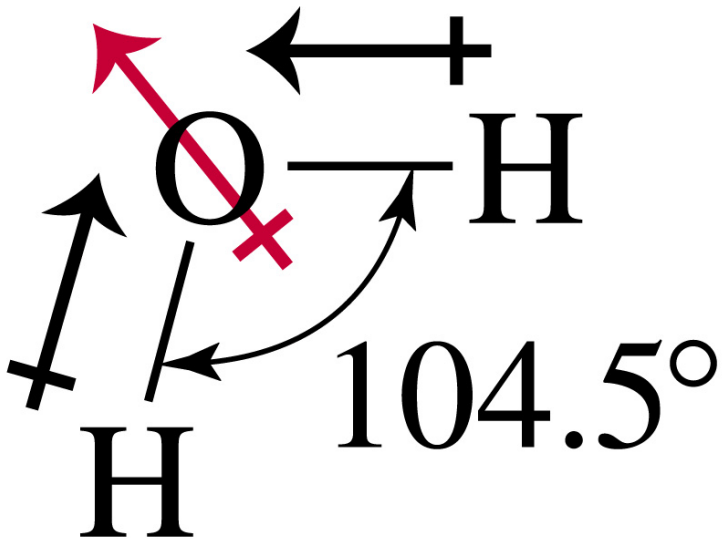


Hybridization

Explains shapes of molecules

CH_4 why are all four C H bonds equal length ?

Electron configurations would suggest bonds not all equal

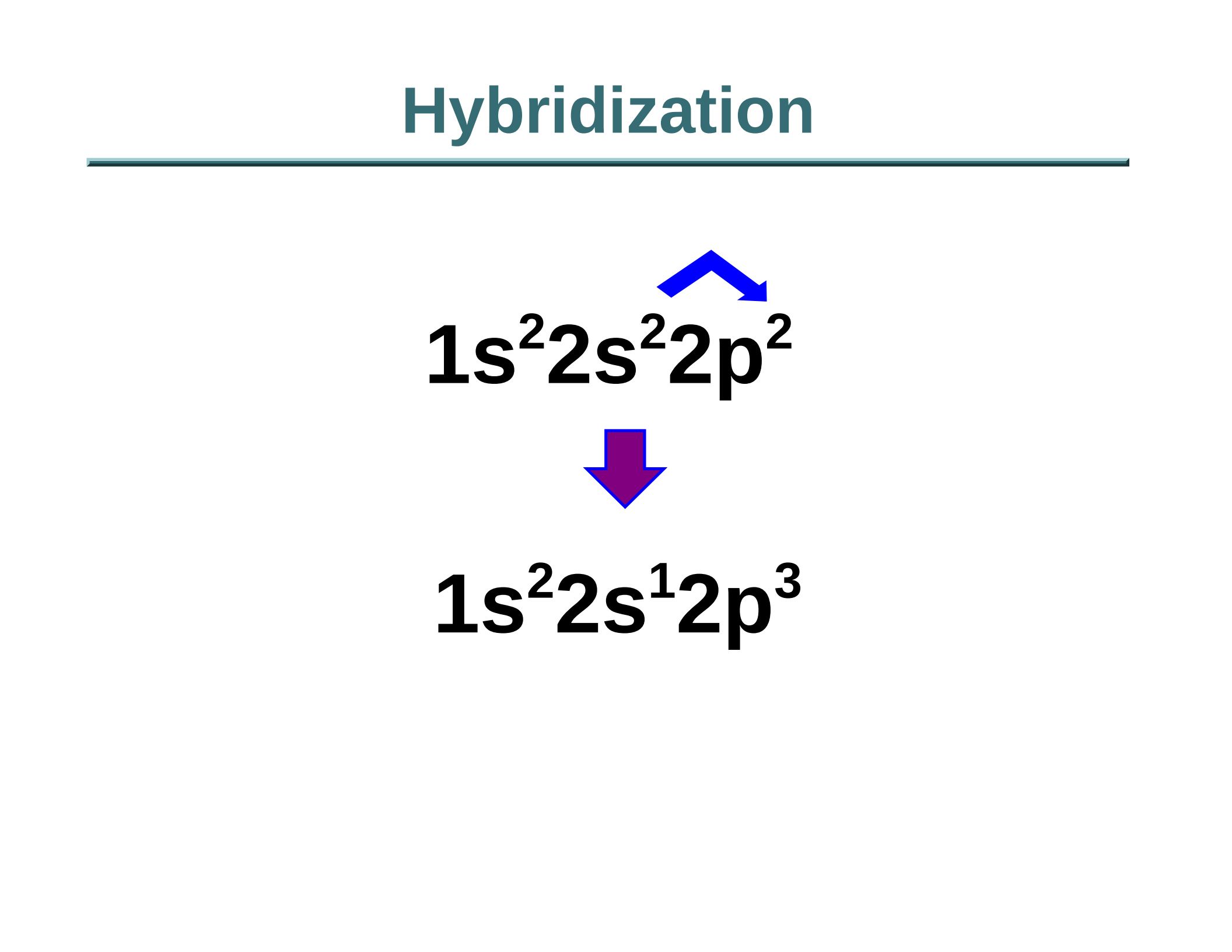
Hybridization

$_{6}C: 1s^2 2s^2 2p^2$

overlaps with four

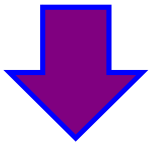
$_{1}H: 1s^1$

Hybridization



Hybridization

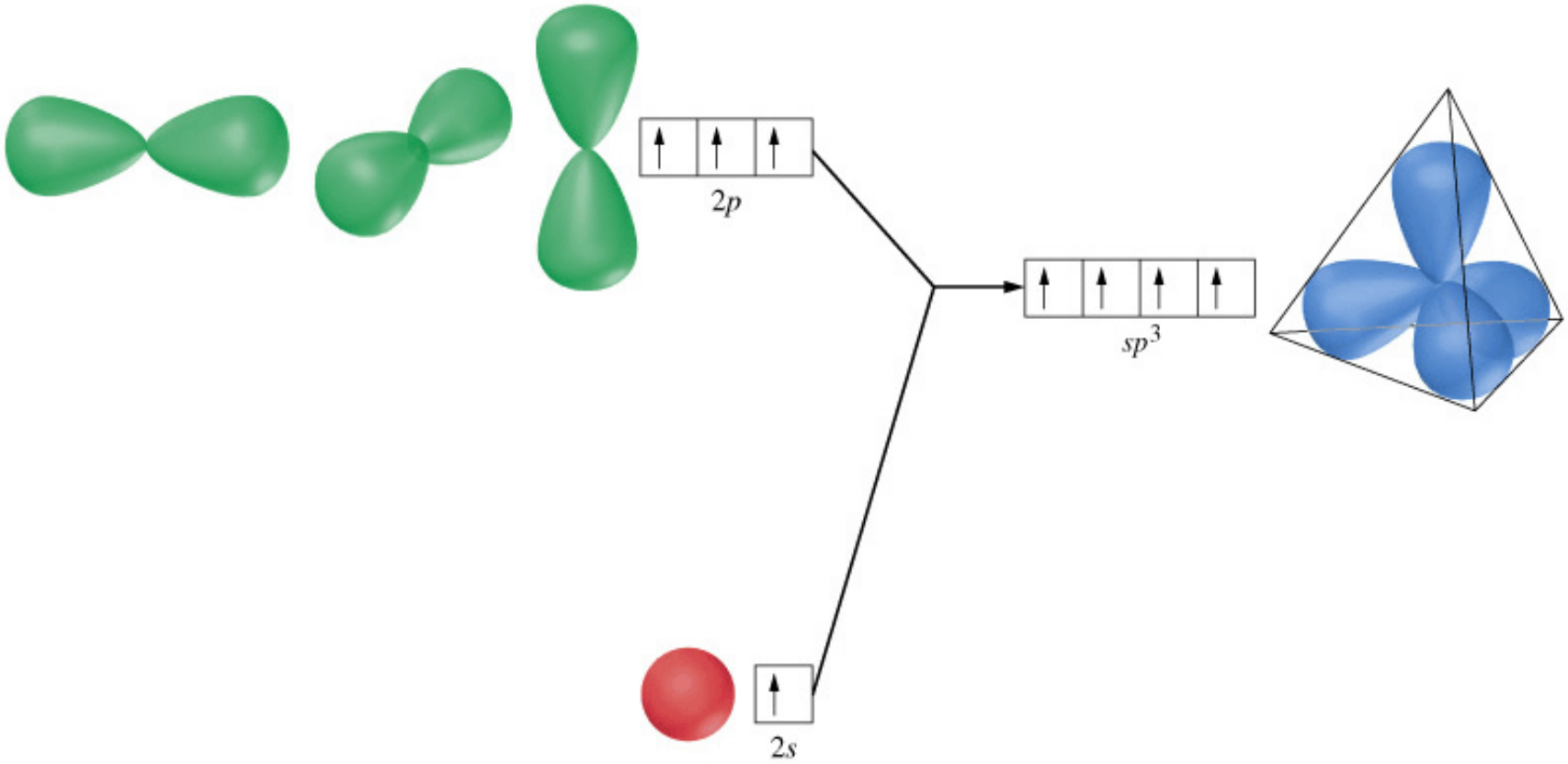
$1s^2 2s^2 2p^2$



$1s^2 2s^1 2p^3$

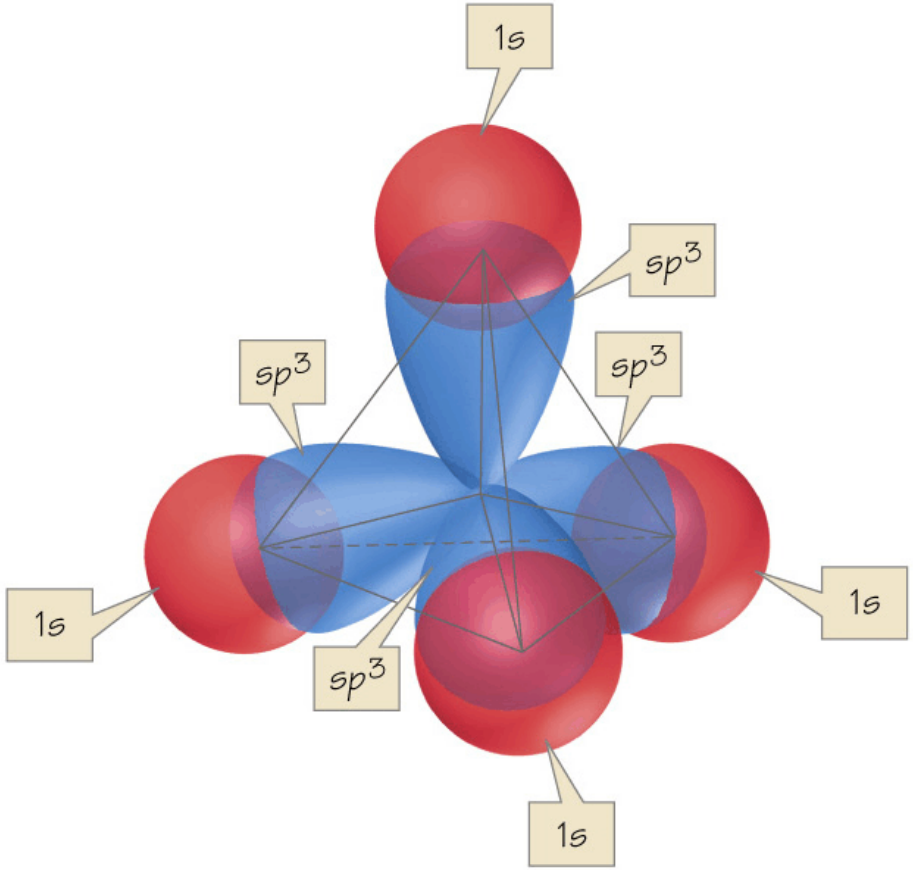
forms sp^3 hybrid orbitals

Hybridization



forms sp^3 hybrid orbitals

Hybridization



forms sp^3 hybrid orbitals