Chapter 9
Molecular Geometries

and Bonding Theories

Coverage of Chapter 9

9.1 All

9.2 All

9.3 All

9.4 All

9.5 Omit Hybridization Involving d Orbitals

9.6 All

9.7 and 9.8 Omit ALL

Molecular Shapes

- The shape of a molecule plays an important role in its reactivity.
- By knowing the number of bonding and nonbonding electron pairs we can predict the shape of the molecule.

Two (2) Theories for MOLECULAR GEOMETRY

1. **V**alence **S**hell **E**lectron **P**air **R**epulsion *(VSEPR) THEORY*

&

2. The **V**alence **B**ond *(VB) THEORY*

Lewis Structures
&
Formal Charge

Formal charge is a charge assigned to each atom in a Lewis structure that helps to distinguish among competing structures.

What is the correct formula for
Hypo Chlorous Acid
$HClO$ (aq)

H – Cl – O

or

H – O – Cl

Hypo chlorite ion
ClO^-

$$|\overline{\underline{O}} - \overline{\underline{Cl}}|$$

	O	Cl
Number of Valence e^-	6	7
Number of Nonbonding e^-	- 6	- 6
½ Number of Bonding e^-	- 1	- 1
Formal Charge	-1	0

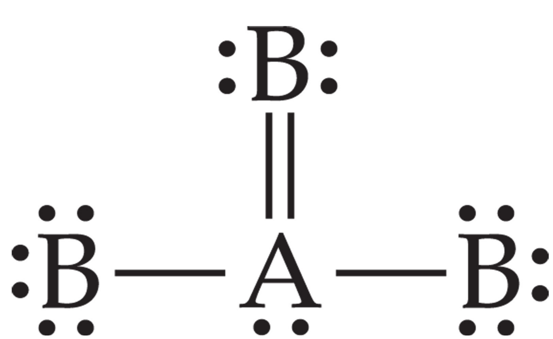
Where does the H go on HClO?

| O – Cl – H   or   H – O – Cl |

	O	Cl	O	Cl
Valence e^-	6	7	6	7
Nonbonding e^-	-6	-4	-4	-6
½ Bonding e^-	-1	-2	-2	-1
	-1	-1	0	0

Electron Domains

- Electron pairs are refered to as electron domains
- Single, double or triple bonds all count as one electron domain.



The atom A in this molecule, has four electron domains.

The First
MOLECULAR GEOMETRY theory
(**VSEPR**)

Valence **S**hell **E**lectron **P**air
Repulsion theory

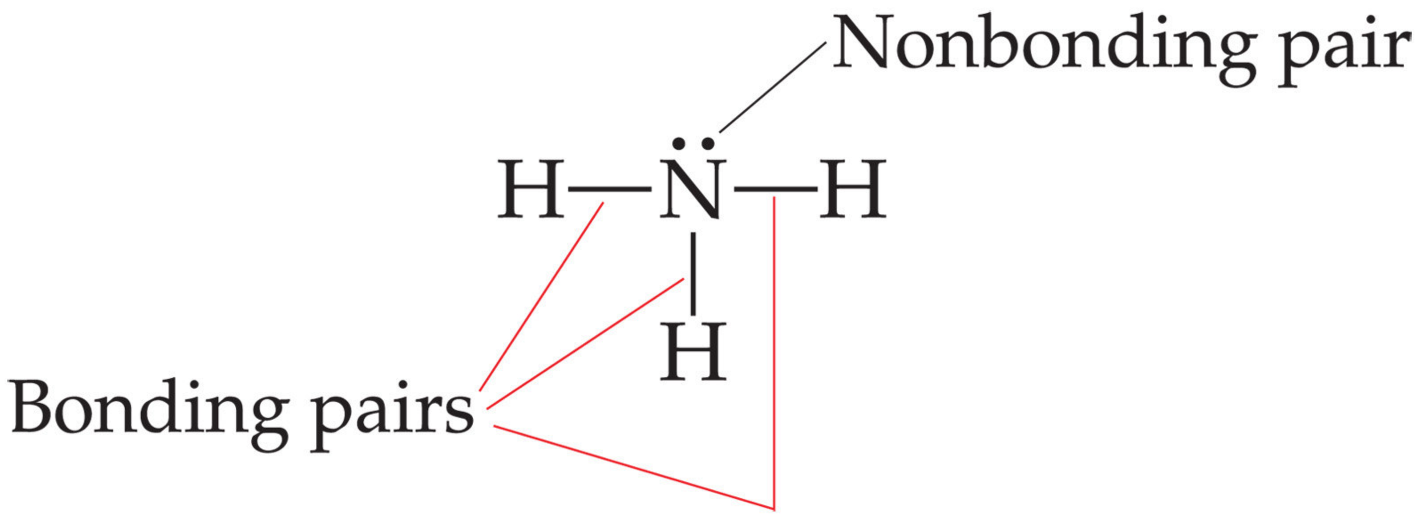
VSEPR Theory

1. To predict molecular shape, assume the valence electrons repel each other

2. The electrons adopt an arrangement in space to minimize e^- e^- repulsion

3. The molecule adopts whichever 3D geometry minimized this repulsion.

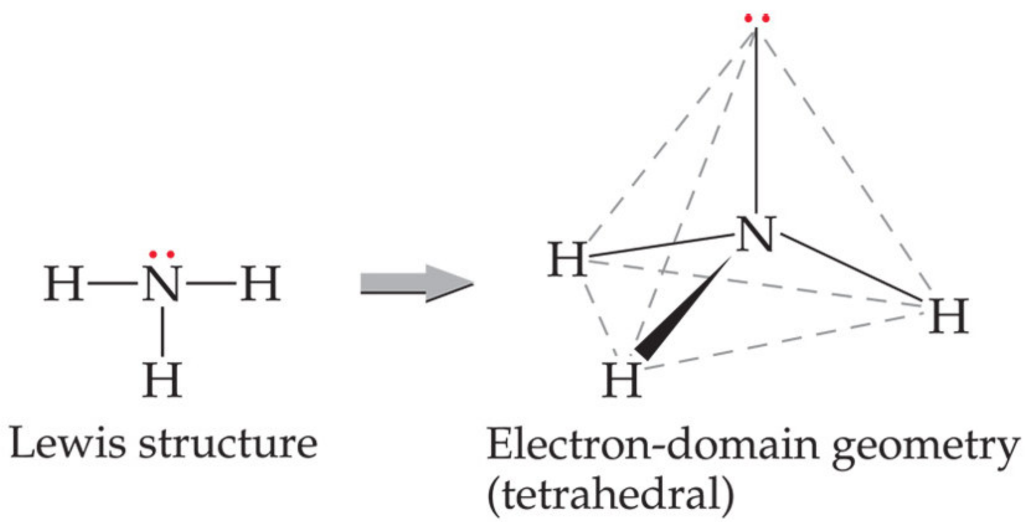
What Determines the Shape of a Molecule?



Four electron domains on N

3 bonding and 1 nonbonding

What Determines the Shape of a Molecule?



Electrons, whether they be bonding or non-bonding, repel each other. So electrons are placed as far as possible from each other

Two (2) Different “Types” of Molecules

1. Molecules with NO nonBonding electrons on the central atom

2. Molecules with nonBonding electrons on the central atom

Electron Domains & NonBonding Electrons

Example 1 CO_2

| O = C = O |

How many electron domains on C 2

How many NonBonding electrons on C 0

Electron Domains & NonBonding Electrons

Example 2 H_2O

..
H – <u>O</u>– H

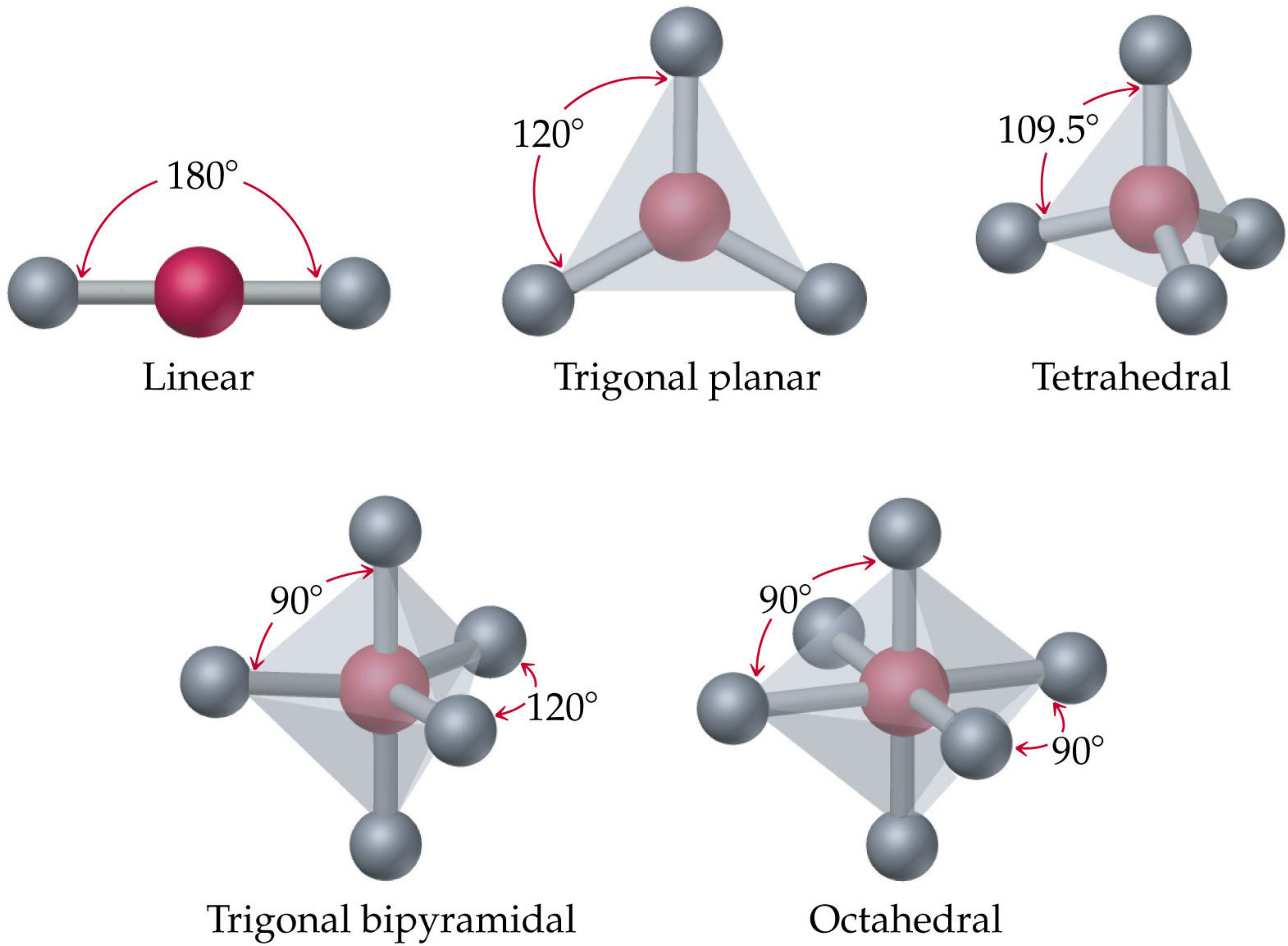
How many electron domains on O 4

How many NonBonding electrons on O 4

Molecular Geometries for molecules with no nonbonding electrons on central atom

There are five fundamental geometries :

1. Linear
2. Trigonal Planar
3. Tetrahedral
4. Trigonal bepyramidal
5. Octahedral


180°
Linear
120°
Trigonal planar
109.5°
Tetrahedral
90°
120°
Trigonal bipyramidal
90°
90°
Octahedral

Only consider Three in detail

1. Linear
2. Trigonal Planar
3. Tetrahedral

In order to determine geometry

First Draw Lewis Dot Formula

MOLECULES IN WHICH THE CENTRAL ATOM HAS NO LONE PAIRS

ZINC CHLORIDE

$ZnCl_2$ Zn (30) [Ar] $3d^{10}4s^2$

$|\overline{\underline{Cl}} - Zn - \overline{\underline{Cl}}|$

B – A – B

AB_2 = LINEAR

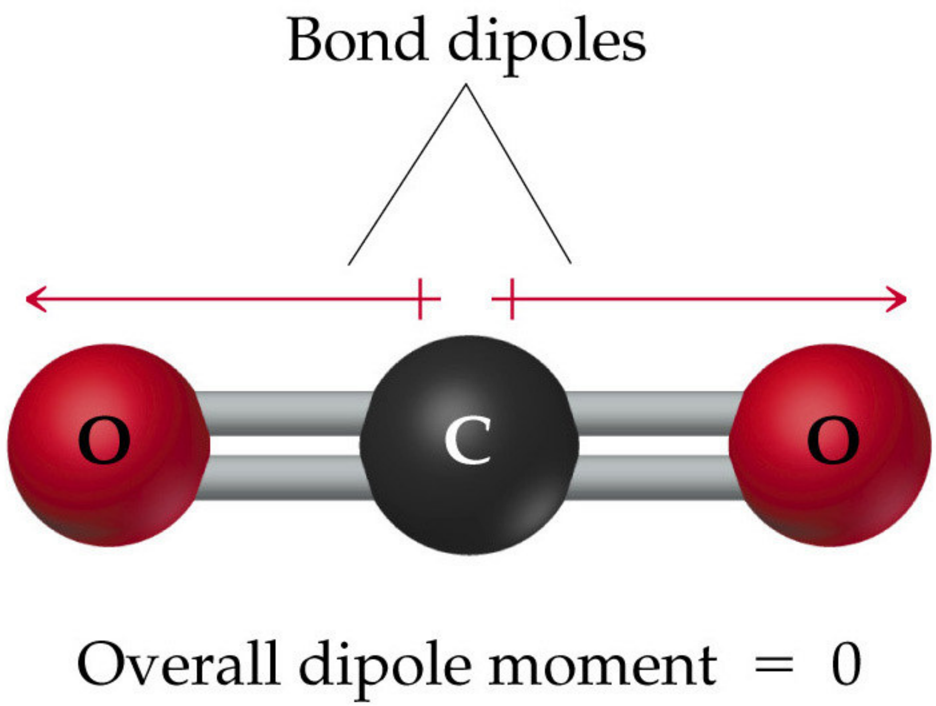
AB_2 Molecules Such as CO_2 are ***<u>Linear</u>***

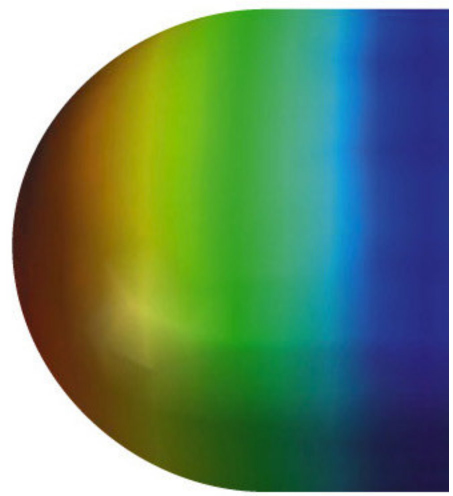
(Molecules With ***NO*** UnPaired Electrons On the Central Atom)

```
 ..         ..
:O = C = O:
```

B – A – B

Molecular Shape and Molecular Polarity





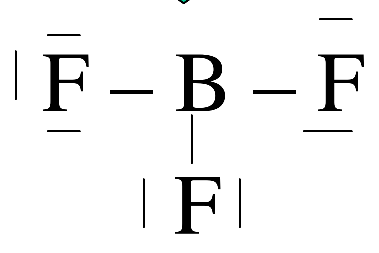
AB_3 Molecules Such as BF_3 are ***Planar***

(Molecules With ***NO*** UnPaired Electrons On the Central Atom)

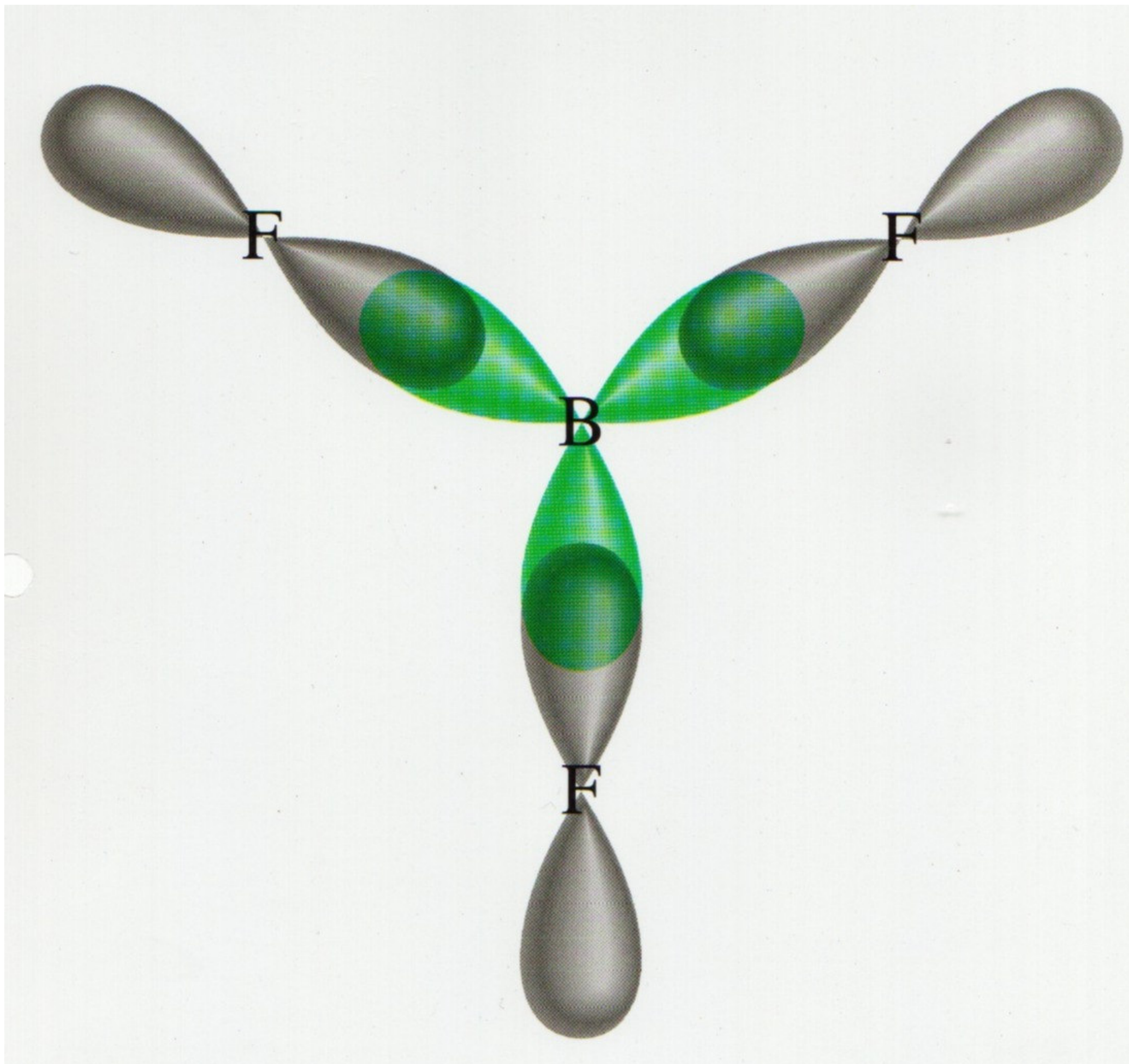
Formula $\quad$ B F_3

Number of Valence e^- $\quad$ 3 $\quad$ 21 = 24 total

- Lewis Structure



AB_3 (Molecules With NO UnPaired Electrons On the Central Atom) Such as BF_3 are Planar



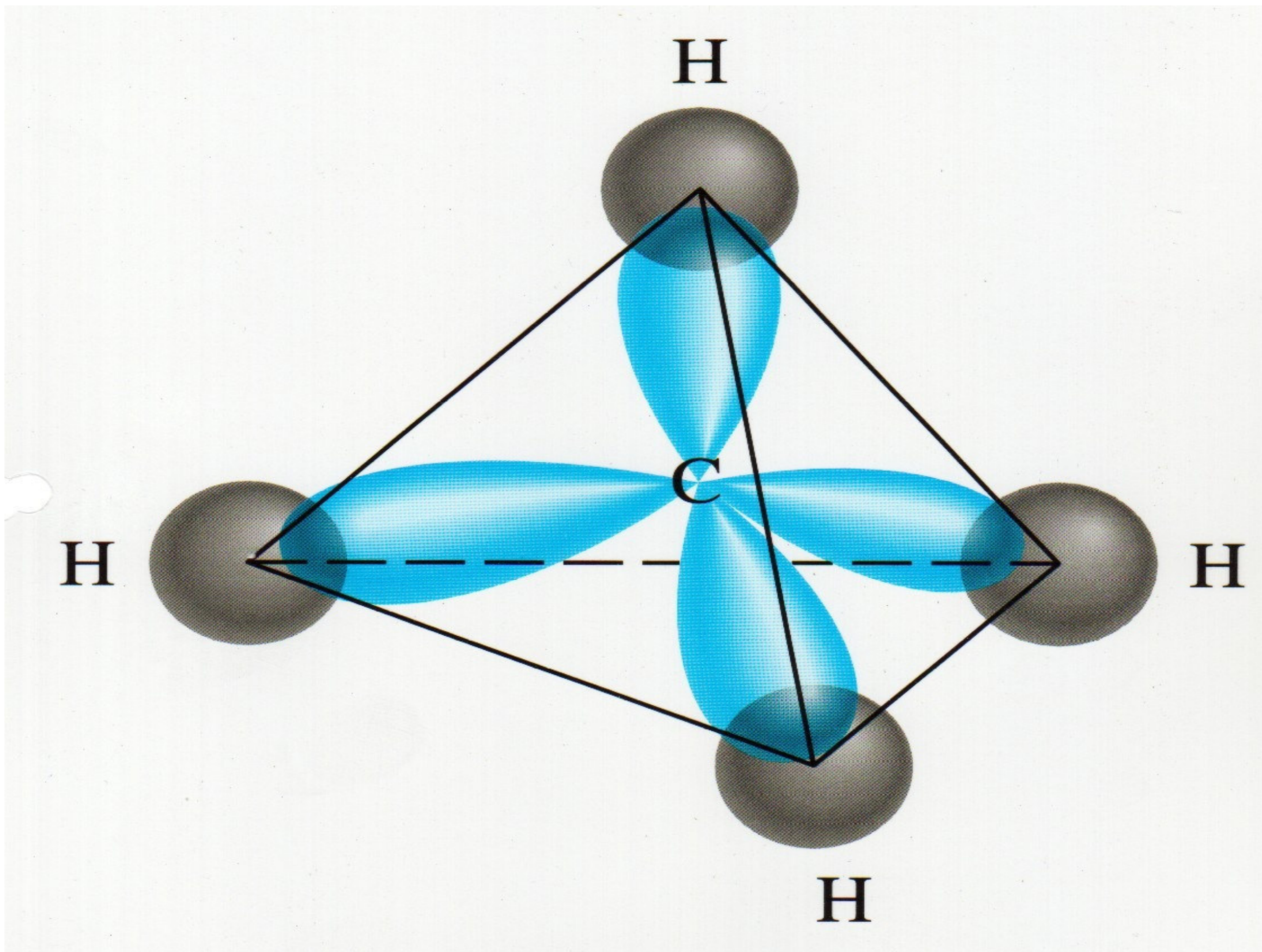
AB_4 Molecules Such as CH_4 are Tetrahedral (Molecules With NO UnPaired Electrons On the Central Atom)

- Formula $C\ H_4$
- Number of Valence e^- 4 4 = 8 total
- Lewis Structure

```
      H
      |
  H – C – H
      |
      H
```

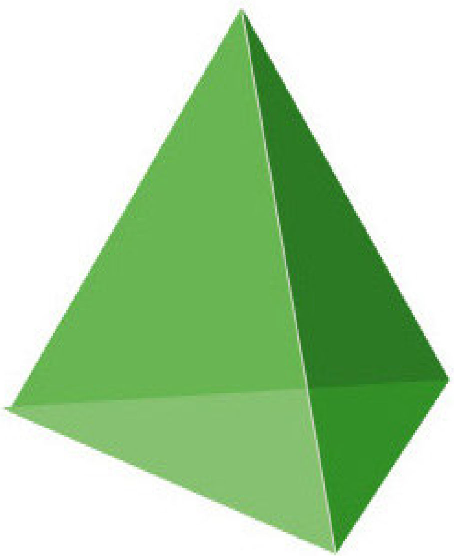
AB_4 Such as CH_4 are Tetrahedral

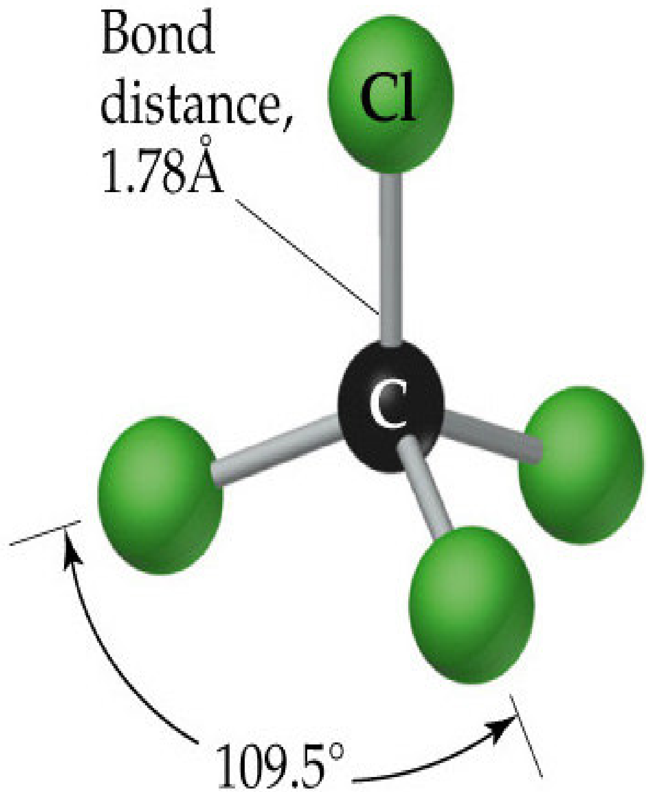
(Molecules With NO UnPaired Electrons On the Central Atom)

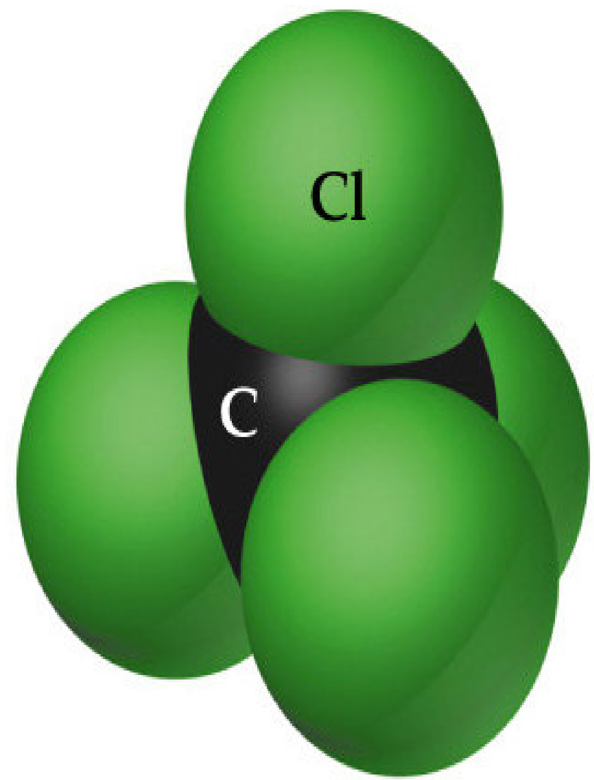


AB_4 Molecules Such as CCl_4 are Tetrahedral

Carbon TetraChloride

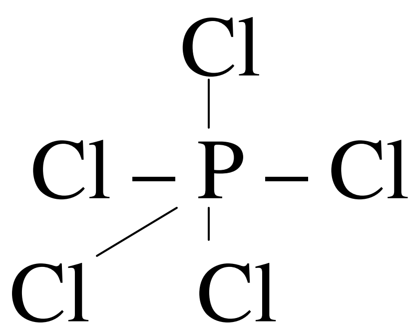






AB_5 Such as PCl_5 are Triangular bipyramidal

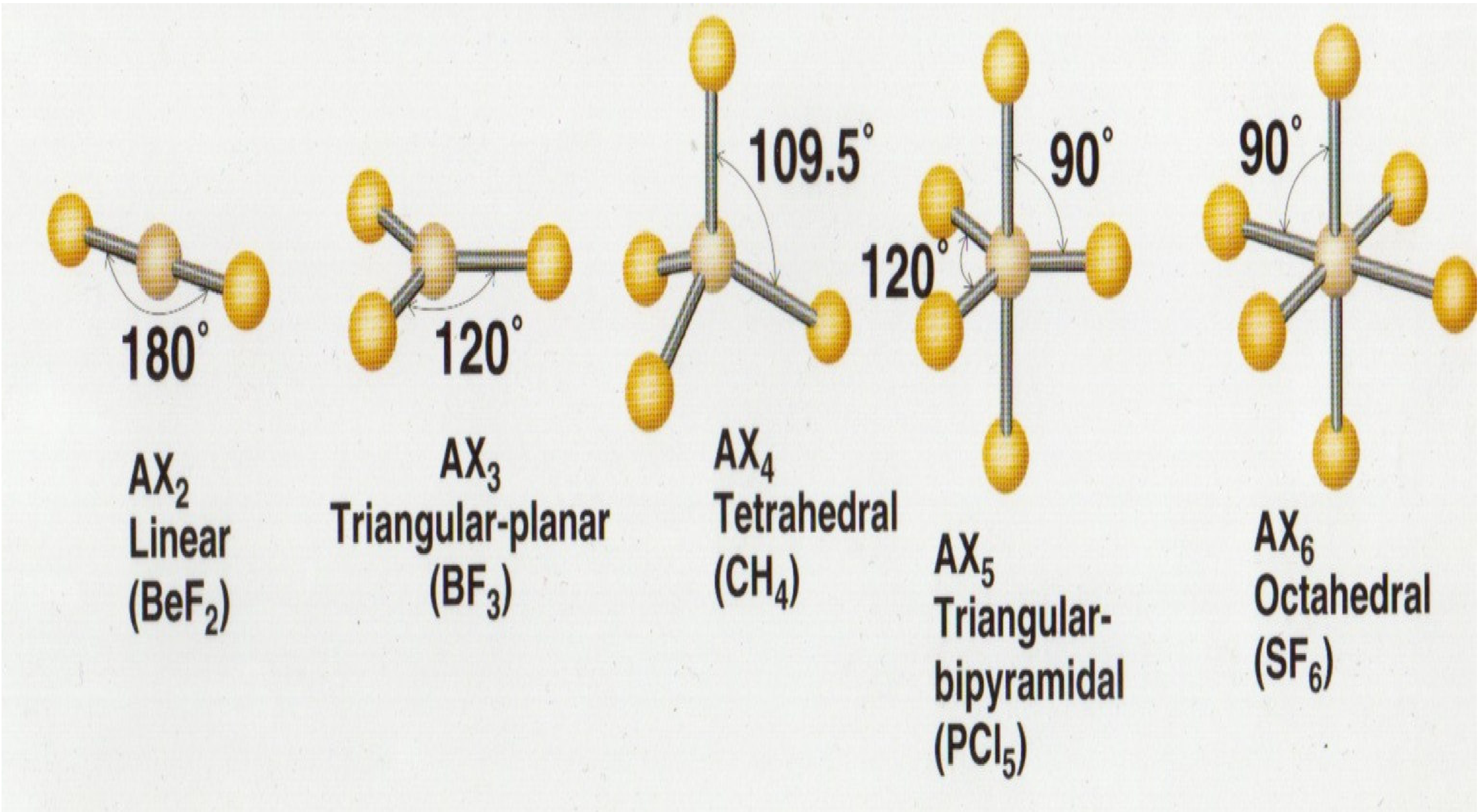
- Name ?
- Number of Bonds ?
- Lewis dot structure ?



AB_6 Such as SF_6 are Octahedral

- Name ?
- Number of Bonds ?
- Lewis dot structure ?

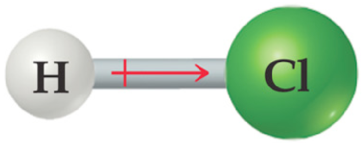
Molecules With NO UNPaired e^-



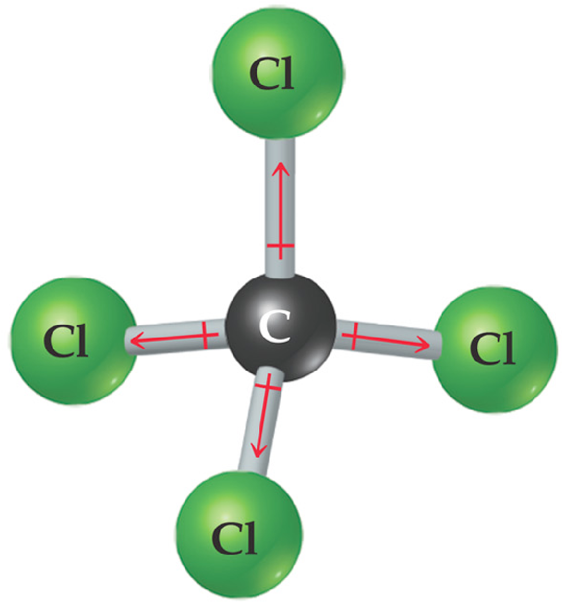
Molecules with NO unpaired e^- on Central Atom

1. 2 Bonds ……….AB_2 or AX_2 e.g. CO_2
2. 3 Bonds ……... AB_3 or AX_3 e.g. BF_3
3. 4 Bonds ……….AB_4 or AX_4 e.g. CH_4
4. 5 Bonds ……... AB_5 or AX_5 e.g. PCl_5
5. 6 Bonds ……... AB_6 or AX_6 e.g. SF_6

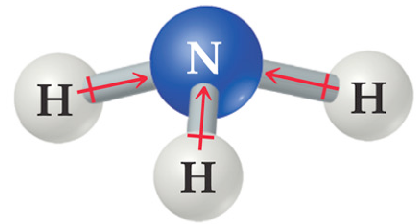
Polarity



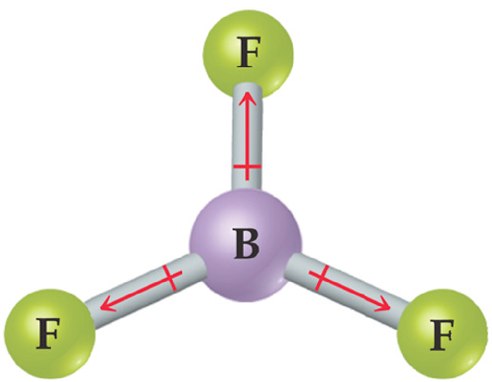
Polar



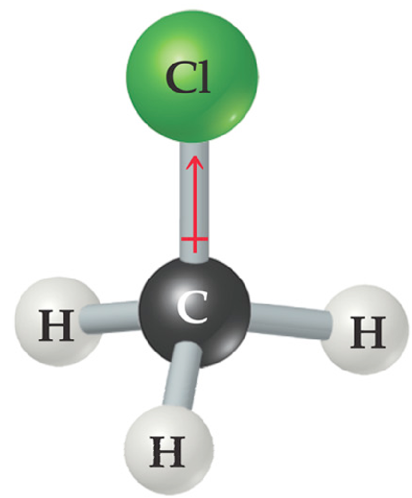
Nonpolar



Polar



Nonpolar



Polar

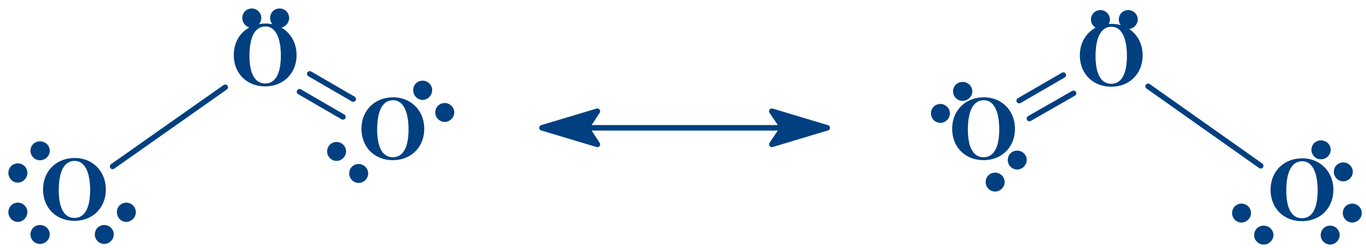
Part 2. of VSEPR Theory

CENTRAL ATOM HAS LONE PAIRS

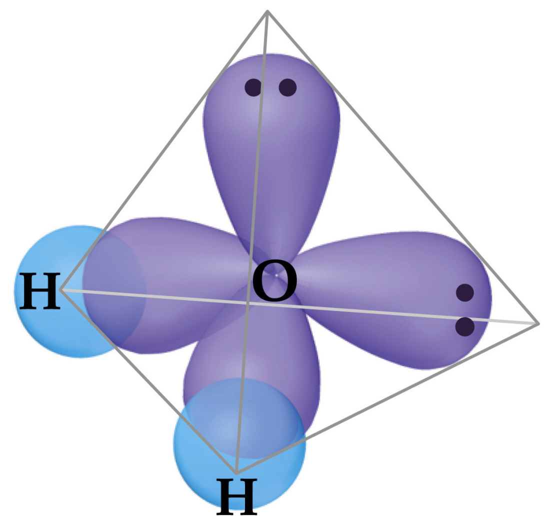
Molecules With UnPaired Electrons On the Central Atom

Class	Example	Geometry
• AB_2E	SO_2 & O_3	Bent
• AB_2E_2	H_2O	Bent
• AB_3E	NH_3	Trigonal pyramidal

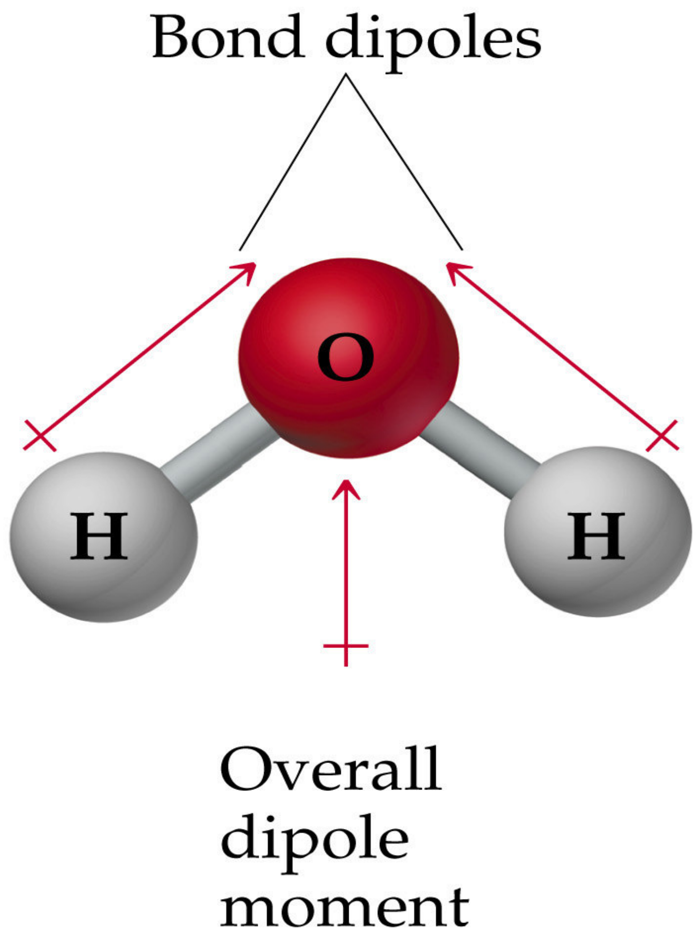
1. AB_2E OZONE

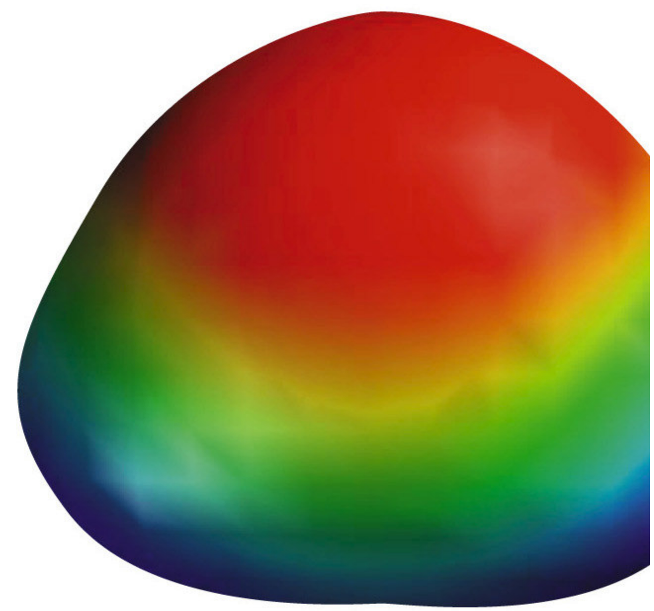


2. AB_2E_2 WATER

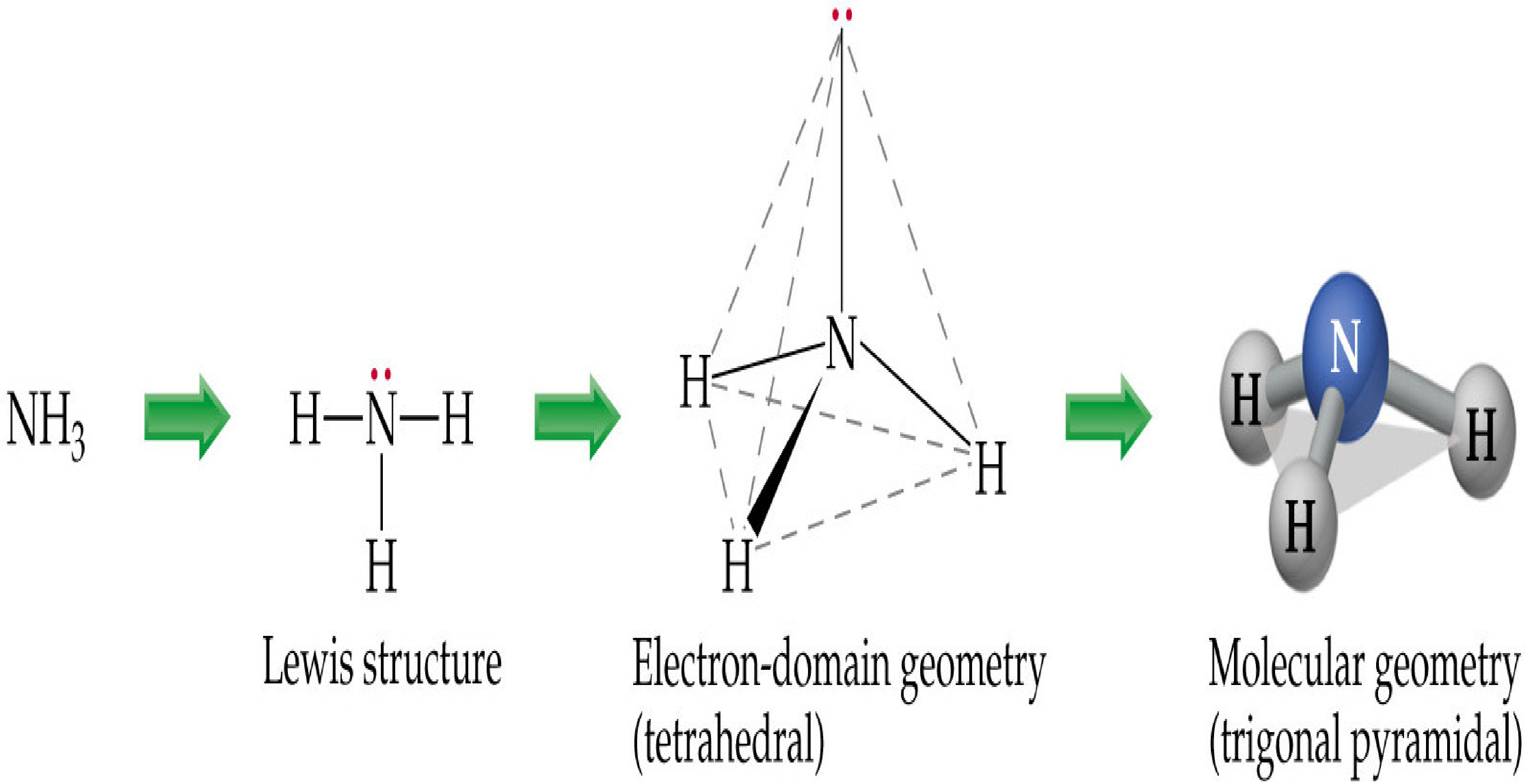


AB_2E_2 (Molecules With UnPaired Electrons On the Central Atom) Such as H_2O are Bent

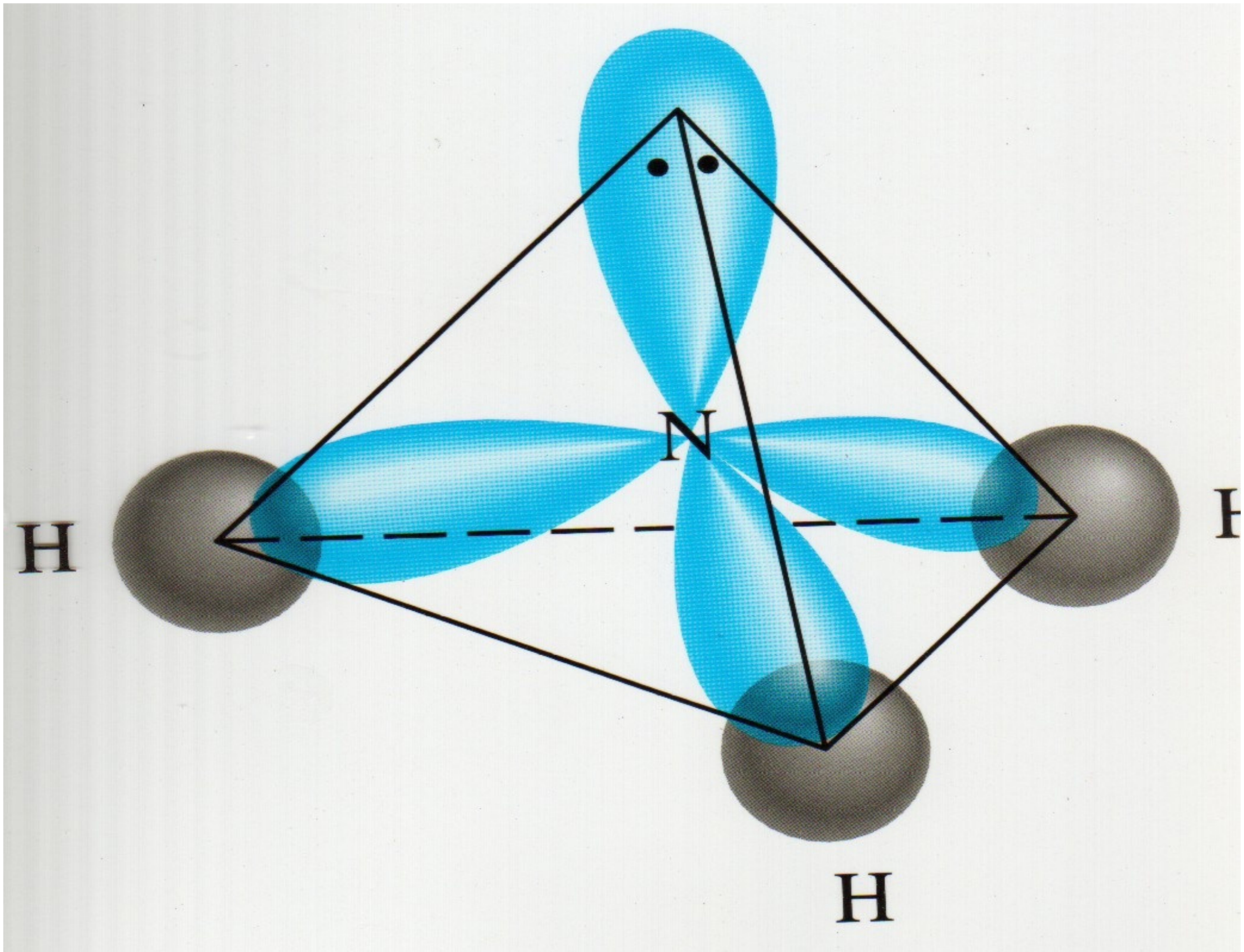




3. AB_3E AMMONIA



AB_3E (Molecules With UnPaired Electrons On the Central Atom) Such as NH_3 are NOT Planar



Predict Molecular Shapes

1. $SiCl_4$ ____________
2. CH_2Cl_2 ____________
3. $GeCl_2$ ____________
4. OF_2 ____________
5. NH_3 _____________
6. PH_3 ______________

Give the
electron domain and molecular geometries for

	electron domain	***molecular geometry***
(a) N_2O	________________	____________________
(b) SO_3	________________	____________________
(c) PCl_3	________________	____________________
(d) NH_2Cl	________________	____________________

Examples of AB_2 molecules

- Linear AB_2 How many bonds

  CO_2

- Bent AB_2E How many "bonds"

  SO_2 and NO_2^-

- Bent AB_2E_2 How many "bonds"

  H_2O

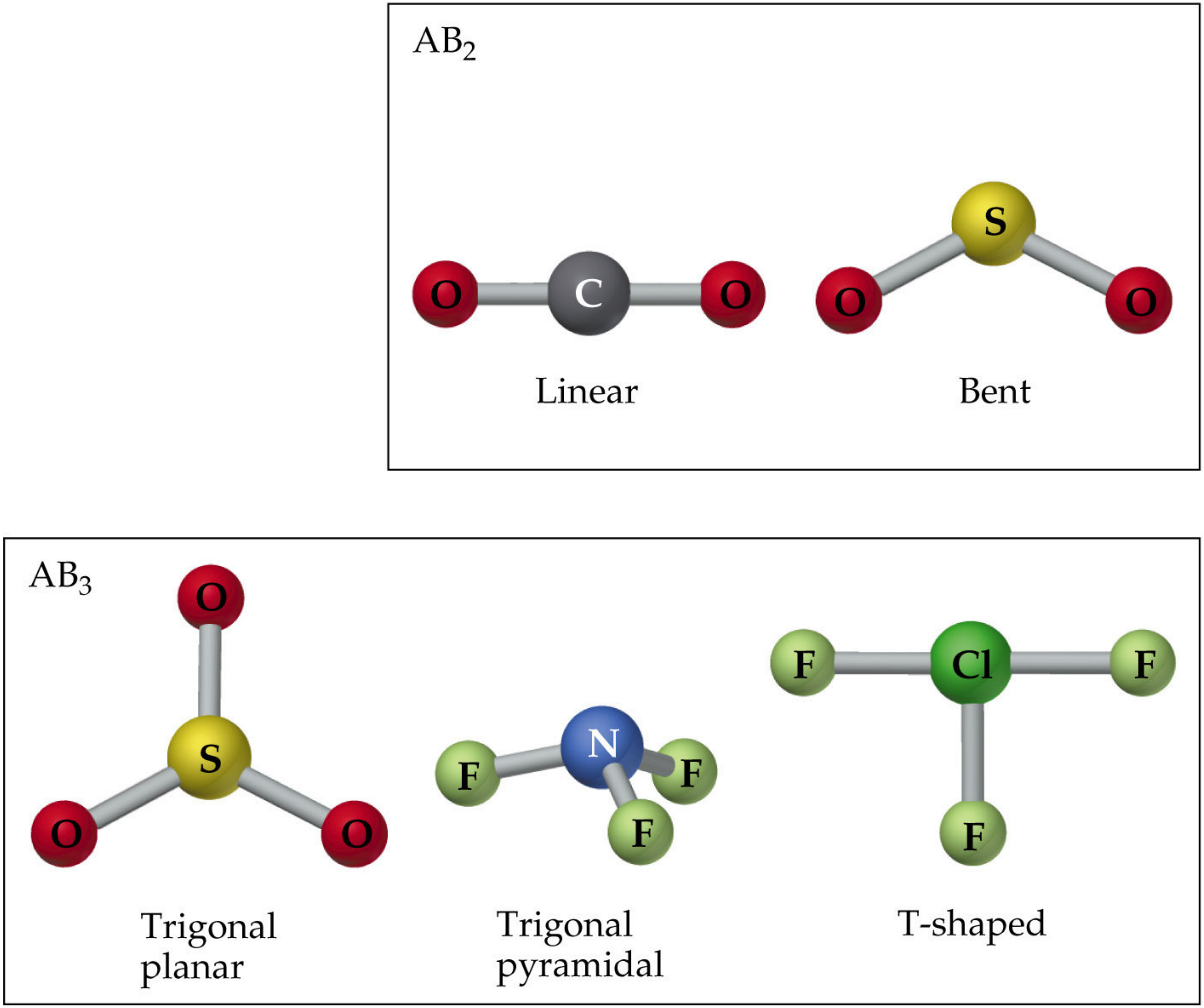
Examples of AB_3 molecules

- Planar AB_3 How many bonds

  BF_3
- Pyramidal AB_3E How many “bonds”

  NH_3
- T shape AB_3E_2 How many “bonds”

  ClF_3



AB_2
O
C
O
Linear
S
O
O
Bent
AB_3
O
S
O
O
Trigonal planar
N
F
F
F
Trigonal pyramidal
F
Cl
F
F
T-shaped

Two (2) Theories for
MOLECULAR GEOMETRY

1. Valence **S**hell **E**lectron **P**air **R**epulsion

(VSEPR) THEORY

Now consider

2. The **V**alence **B**ond

(VB) THEORY

VALENCE BOND Method

uses molecular orbitals

not Atomic Orbitals

WHAT IS A MOLECULAR ORGITAL?

Orbitals used in bonding of Molecules

CH_4 as an EXAMPLE

Ground State Electron Configuration

C (6 e^-) $1s^2\ 2s^2\ 2p^2$ = (↑↓) (↑↓) (↑) (↑) ( )

Only place for two bonds to form ⇧ ⇧

Therefore would predict CH_2 formation and not CH_4

But CH_2 does not exist while CH_4 does

C (6 e^-) $1s^2\ 2s^2\ 2p^2$ = $(\uparrow\downarrow)\ (\uparrow\downarrow)\quad (\uparrow)\ (\uparrow)\ (\ )$

Only place for two bonds to form

Excited State Electron Configuration

C (6 e^-) $1s^2\ 2s^1\ 2p^3$ = $(\uparrow\downarrow)\ (\uparrow)\quad (\uparrow)\ (\uparrow)\ (\uparrow)$

Now a place for four bonds

One electron from H goes into an s orbital

and Three from H go into the p orbitals

The **BONDS** in CH_4 are **ALL** the **SAME!**

One electron in an s orbital and Three in p orbitals would create different bonds.

Since All the Bonds are Equal, this cannot be correct

INTRODUCE THE CONCEPT OF HYBRIDIZATION

Hybridization

In order to made All Bonding sites equal, we must create NEW Orbitals.

s, p, d, f are ATOMIC ORBITALS

MOLECULAR ORBITALS are formed from Atomic orbitals

VALENCE BOND THEORY

VALENCE SHELL ORBITALS *HYBRIDIZE*

THE ORIENTATION OF ALL HYBRID VALENCE SHELL ORBITALS DETERMINES THE GEOMETRY OF THE MOLECULE

MOLECULAR ORBITALS
are formed from
ATOMIC ORBITALS

Atomic Orbitals	Molecular Orbitals
one S + one P	Two (2) SP
one S + two P	Three (3) SP^2
one S + three P	Four (4) SP^3

MOLECULAR ORBITALS

They are called

SP

SP^2

SP^3

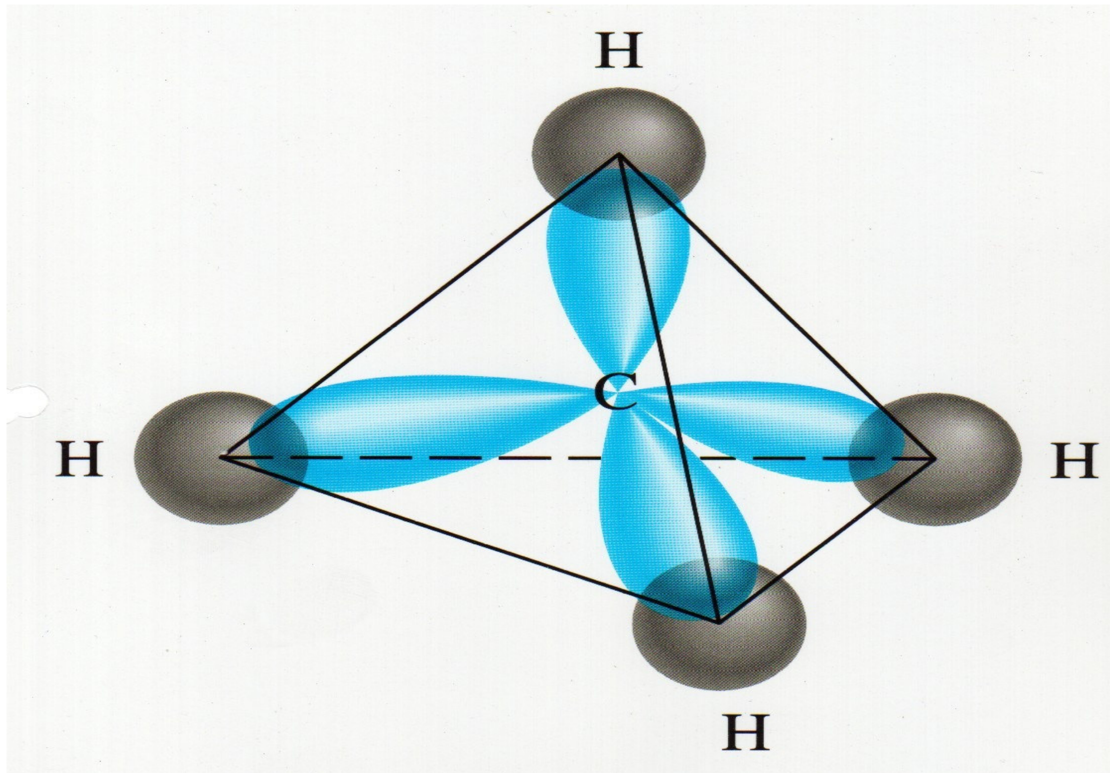
SP^3d and

SP^3d^2

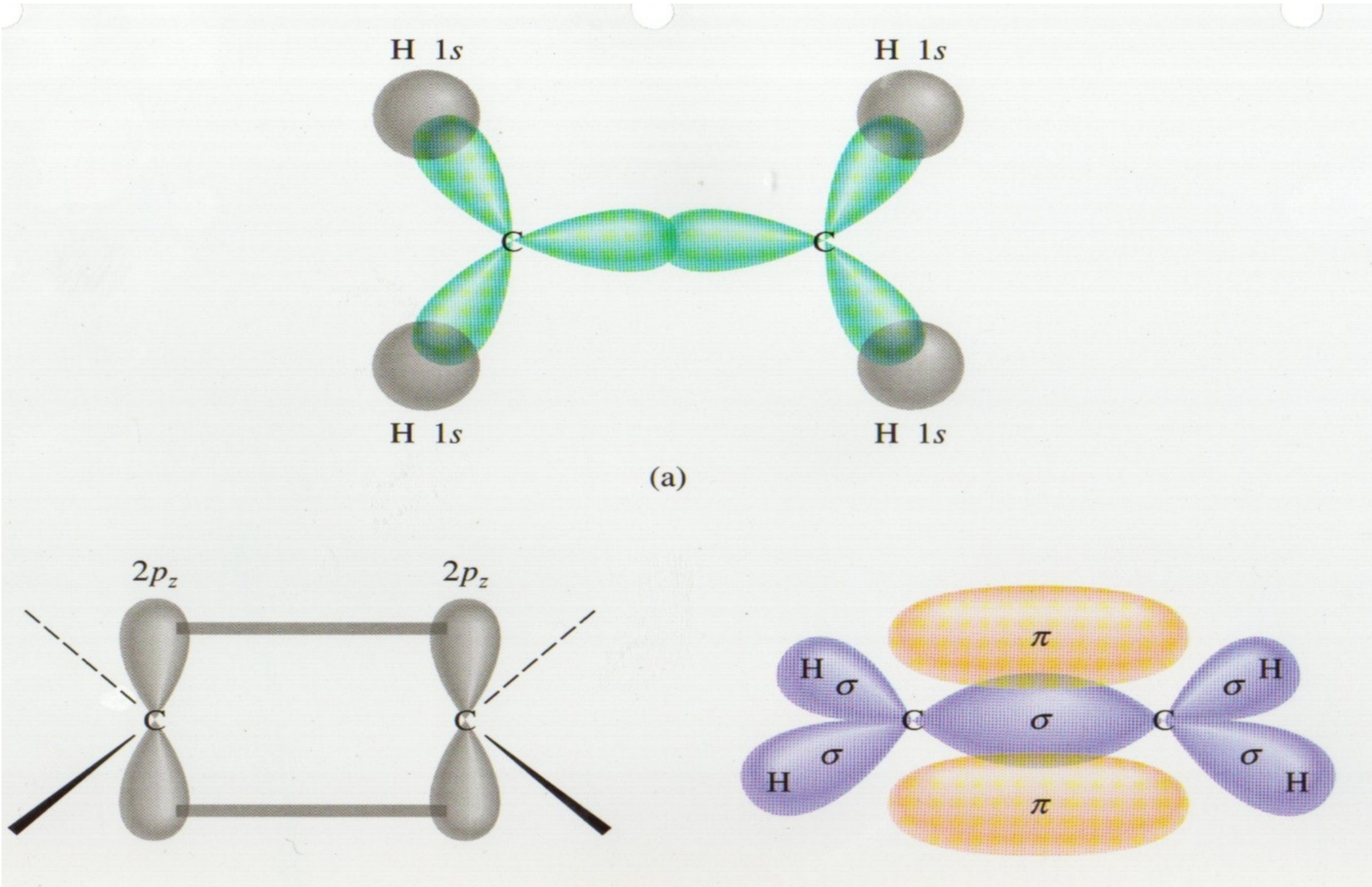
sp^3 HYBRIDIZATION

TETRAHEDRAL
Bond Angles
109½°

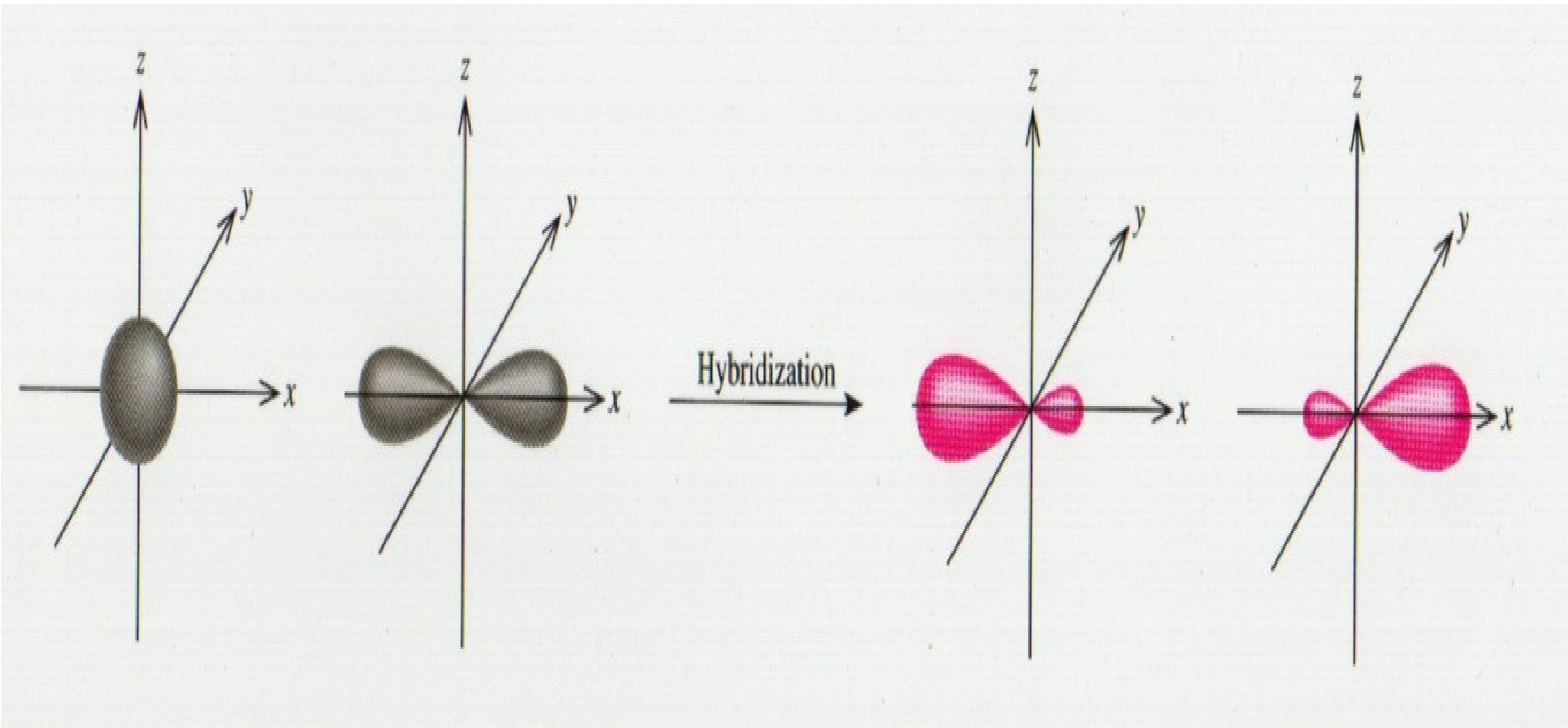
Methane CH_4
Four σ Bonds
on C



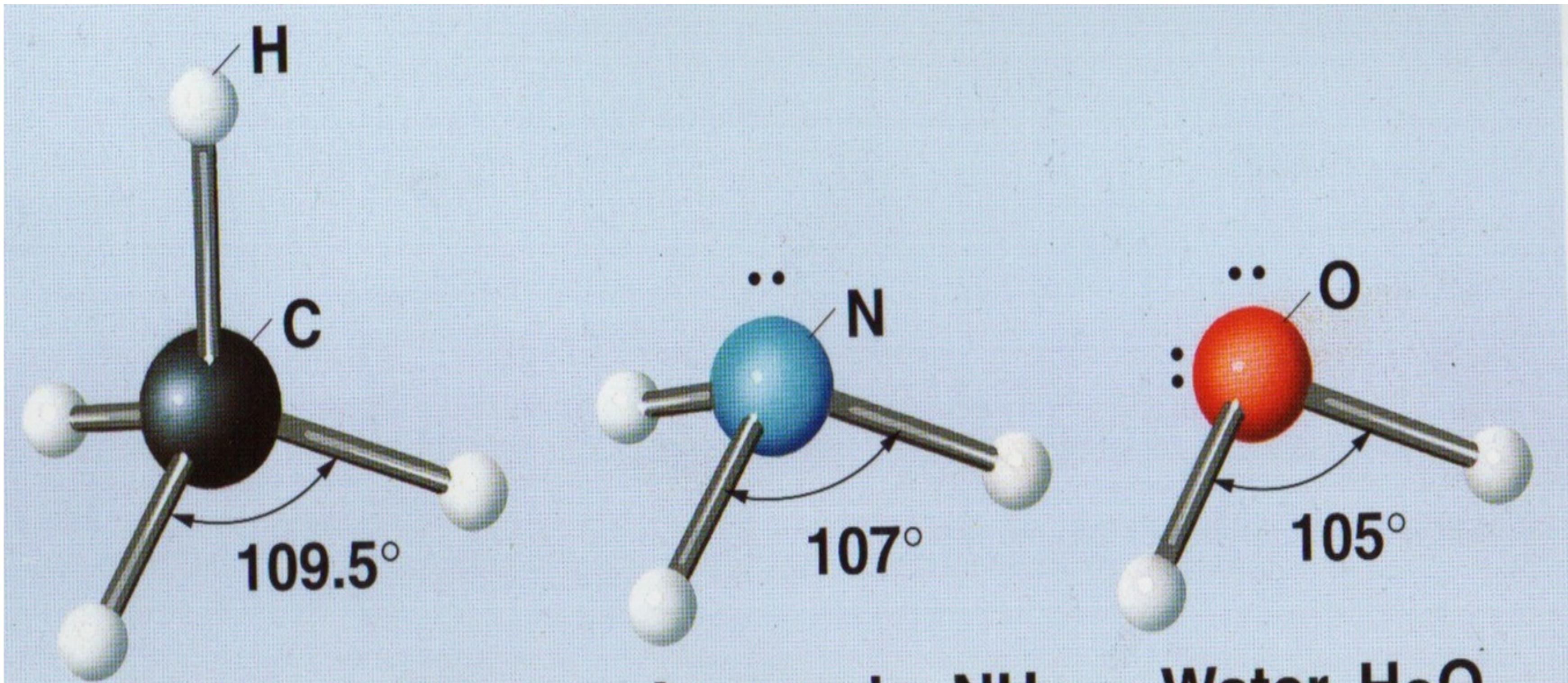
sp^2 HYBRIDIZATION



sp HYBRIDIZATION
one S orbital + one P orbital



Carbon is NOT The Only Element That Undergoes sp^3 HYBRIDIZATION



Methane, CH_4
4 bond pairs

Ammonia, NH_3
3 bond pairs

Water, H_2O
2 bond pairs

In CH_3COOH, there are three (3) hybridized atoms.
Geometry is assign about each hybridized atom separately.