

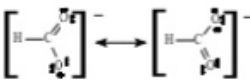
# Chemical Bonds

Section \_\_\_\_\_

Name \_\_\_\_\_

## Report Sheet

Complete the table following the pattern given in the example.

3-D molecular drawing, with Lewis resonance structures, if necessary	VSEPR geometry, $AB_xE_y$ hybridization	Molecular shape, bond angles	Polarity, bond lengths
$\text{HCO}_2^-$ 	Trigonal planar $AB_3E_0$ Carbon is $sp^2$ hybridized	Trigonal planar $\text{HCO} = 120^\circ$ $\text{OCO} = 120^\circ$	Polar $\text{C-O} = 1.23\text{\AA}$ $\text{H-C} = 1.14\text{\AA}$
$\text{CF}_4$			
$\text{CHI}_3$			
$\text{HCl}$			

1. chemical bond:

-ionic bond:

-covalent bond:

-Electronegativity

-Polar Covalent

2. octet rule:

EXCEPTIONS

3. Lewis dot structure

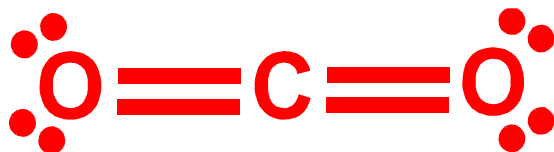
4. Formal Charge:

5. Resonance:

Isomers:

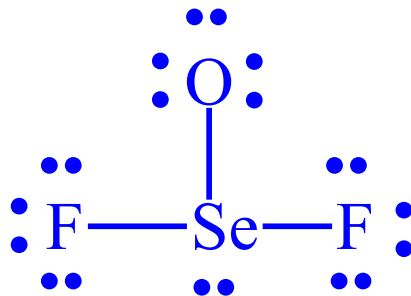
# Practice - Lewis Structures

- $\text{CO}_2$  16  $e^-$



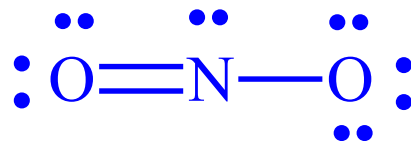
- $\text{SeOF}_2$

26  $e^-$



- $\text{NO}_2^{-1}$

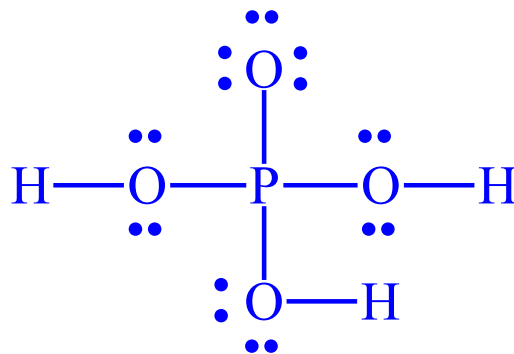
18  $e^-$



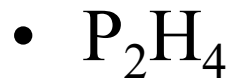
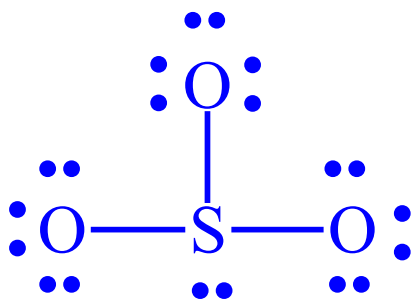
# Practice - Lewis Structures



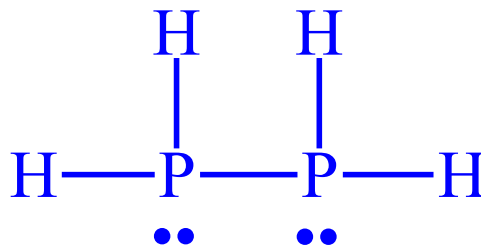
32  $e^-$



26  $e^-$



14  $e^-$



# FORMAL CHARGE

**Formal charge is the “charge” assigned to an atom in a molecule, (1) assuming equal sharing of the electrons & (2) without considering electronegativity effects.**

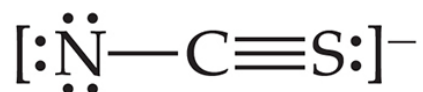
$$\text{FC(X)} = \text{\#VE} - (1/2 \text{ BE} + \text{NBE})$$

**“Formal Charge of (element in compound) = # valence electrons for element – (1/2 bonding electrons + nonbonding electrons)”**

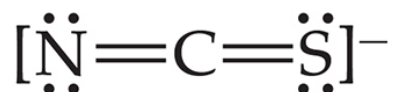
# Writing Lewis Structures

- The dominant Lewis structure:
  - is the one in which atoms have formal charges closest to zero.
  - puts a negative formal charge on the most electronegative atom.
- As such, it can be used to decide which structure is best.
- $N = 5 - (\frac{1}{2}(2) + 6) = -2$
- $C = 4 - (\frac{1}{2}(8) + 0) = 0$
- $S = 6 - (\frac{1}{2}(6) + 2) = +1$

-2    0    +1



-1    0    0



0    0    -1

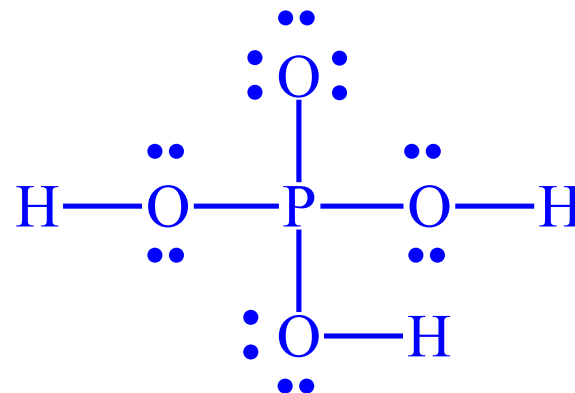


# Practice - Assign Formal Charges

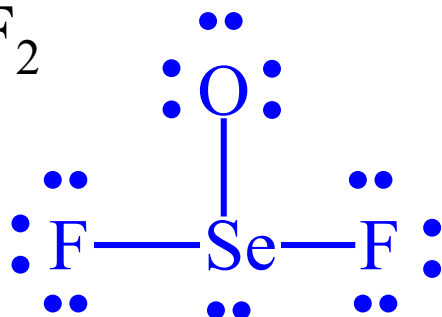
- $\text{CO}_2$



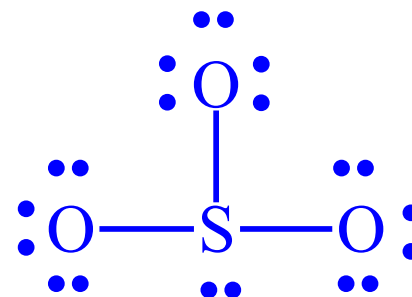
- $\text{H}_3\text{PO}_4$



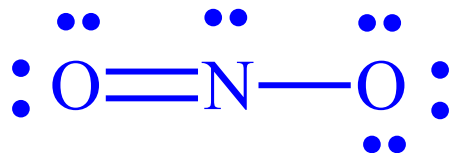
- $\text{SeOF}_2$



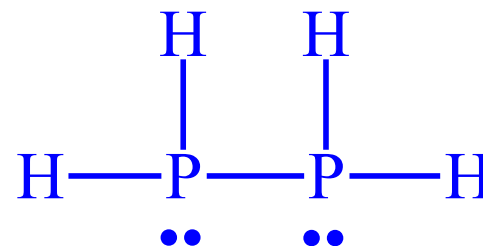
- $\text{SO}_3^{-2}$



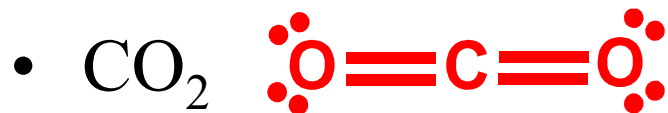
- $\text{NO}_2^{-1}$



- $\text{P}_2\text{H}_4$

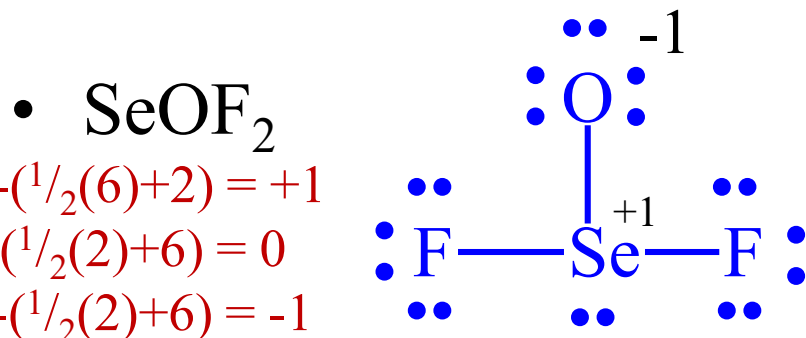


# Practice - Assign Formal Charges



$$\text{O} = 6 - (\frac{1}{2}(4) + 4) = 0$$

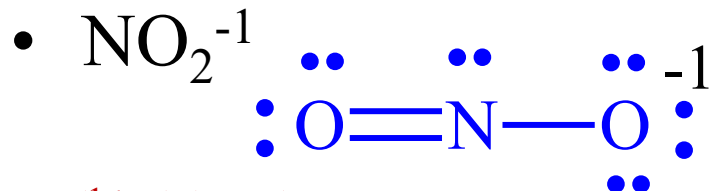
$$\text{C} = 4 - (\frac{1}{2}(8)) = 0$$



$$\text{Se} = 6 - (\frac{1}{2}(6) + 2) = +1$$

$$\text{F} = 7 - (\frac{1}{2}(2) + 6) = 0$$

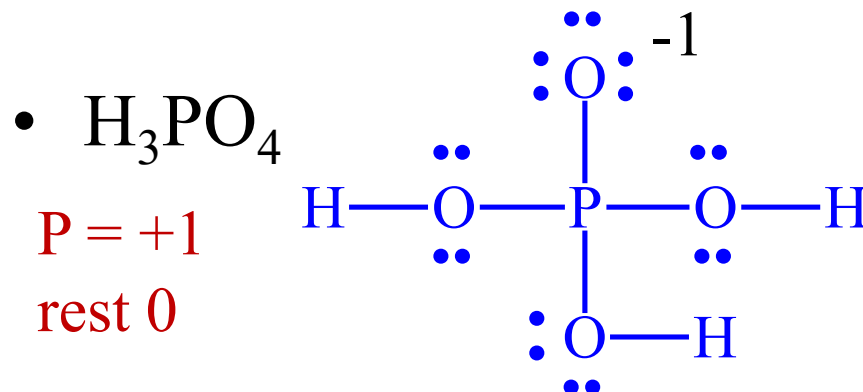
$$\text{O} = 6 - (\frac{1}{2}(2) + 6) = -1$$



$$\text{N} = 5 - (\frac{1}{2}(6) + 2) = 0$$

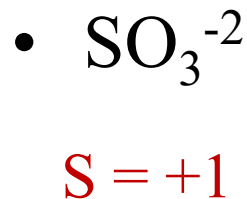
$$\text{O} = 6 - (\frac{1}{2}(4) + 4) = 0$$

$$\text{O} = 6 - (\frac{1}{2}(2) + 6) = -1$$

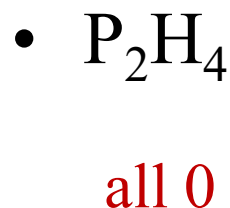


$$\text{P} = +1$$

$$\text{rest } 0$$



$$\text{S} = +1$$



$$\text{all } 0$$

## FORMAL CHARGE EXAMPLE

Predict the most stable structure:  $\text{ONC}^-$  or  $\text{OCN}^-$  or  $\text{NOC}^-$



1) Total electrons is:

$(6e^- \text{ for O}) + (5e^- \text{ for N}) + (4e^- \text{ for C}) + (1e^- \text{ for negative charge}) = 16 e^-$  total. All structures fulfill the octet rule.

2)  $\text{FC (X)} = \# \text{ of valence electrons} - (1/2 \text{ bonding electrons} + \text{nonbonding electrons})$

structure#1:

$$\text{FC(C)} = 4 - (1/2 \cdot 4 + 4) = -2$$

$$\text{FC(O)} = 6 - (1/2 \cdot 4 + 4) = 0$$

$$\text{FC(N)} = 5 - (1/2 \cdot 8 + 0) = +1$$

structure#2:

$$\text{FC(C)} = 4 - (1/2 \cdot 8 + 0) = 0$$

$$\text{FC(O)} = 6 - (1/2 \cdot 4 + 4) = 0$$

$$\text{FC(N)} = 5 - (1/2 \cdot 4 + 4) = -1$$

structure #3:

$$\text{FC(C)} = 4 - (1/2 \cdot 4 + 4) = -2$$

$$\text{FC(O)} = 6 - (1/2 \cdot 8 + 0) = +2$$

$$\text{FC(N)} = 5 - (1/2 \cdot 4 + 4) = -1$$

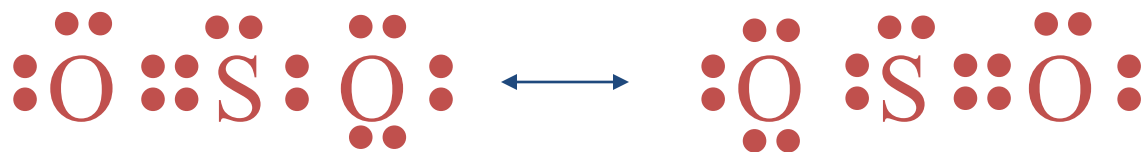
structure #2 has the combination with the lowest formal charge. It also has the negative formal charge on one of the more electronegative atoms. Calculate the formal charge for the most stable structure:





# Resonance

- when there is more than one Lewis structure for a molecule that differ **only** in the position of the electrons, they are called **resonance structures**
- the actual molecule is a combination of the resonance forms – a **resonance hybrid**
  - it does **not** resonate between the two forms, though we often draw it that way
- look for multiple bonds or lone pairs

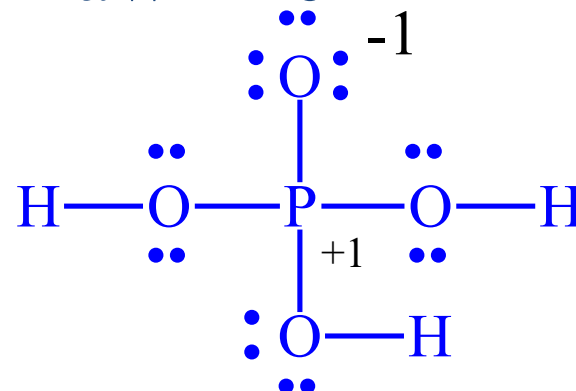


# Practice - Identify Structures with Better or Equal Resonance Forms and Draw Them

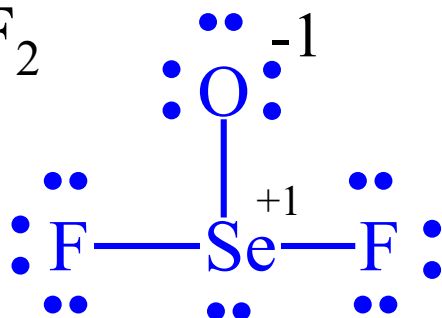
- $\text{CO}_2$



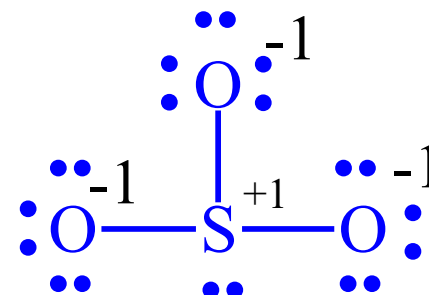
- $\text{H}_3\text{PO}_4$



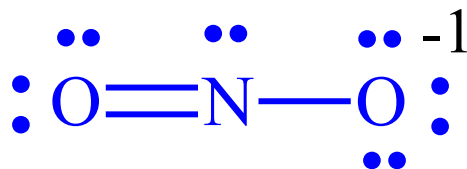
- $\text{SeOF}_2$



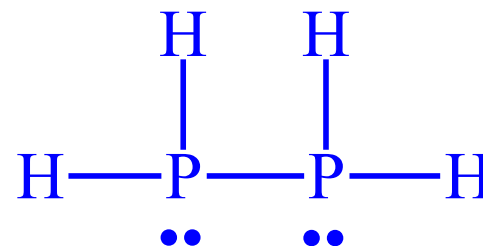
- $\text{SO}_3^{-2}$



- $\text{NO}_2^{-1}$



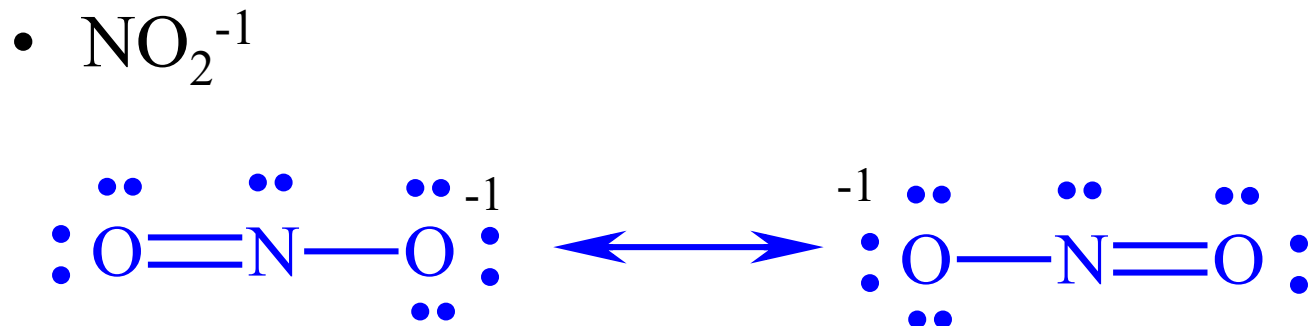
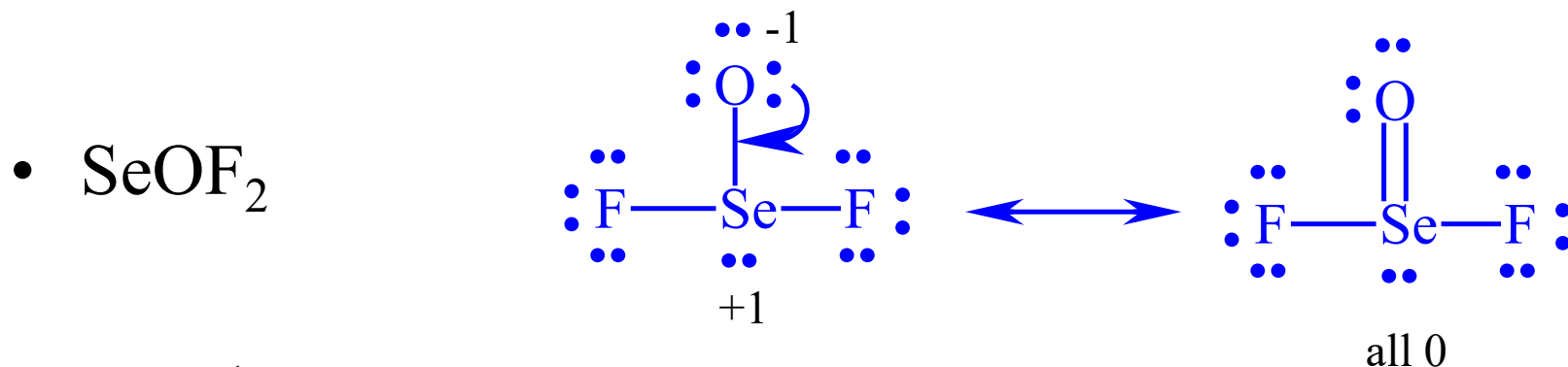
- $\text{P}_2\text{H}_4$



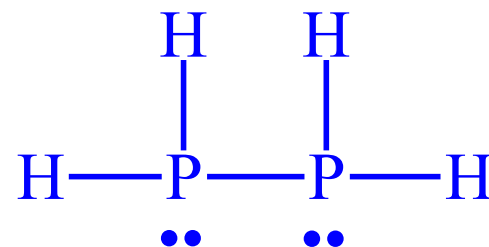
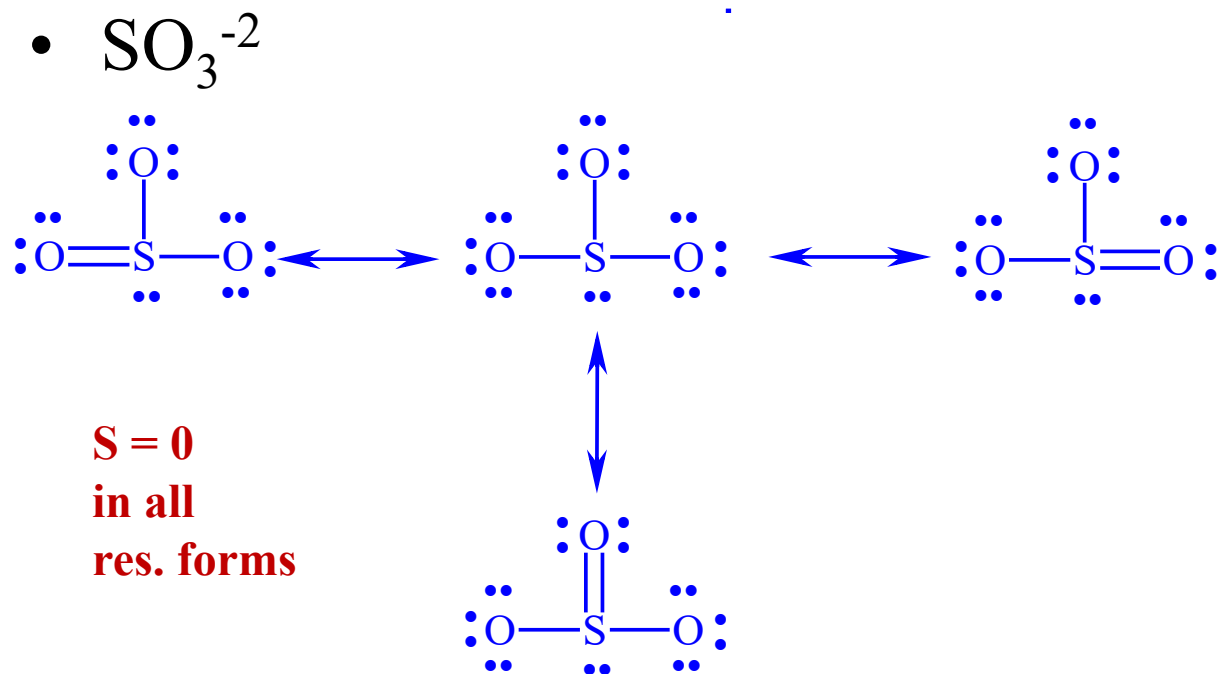
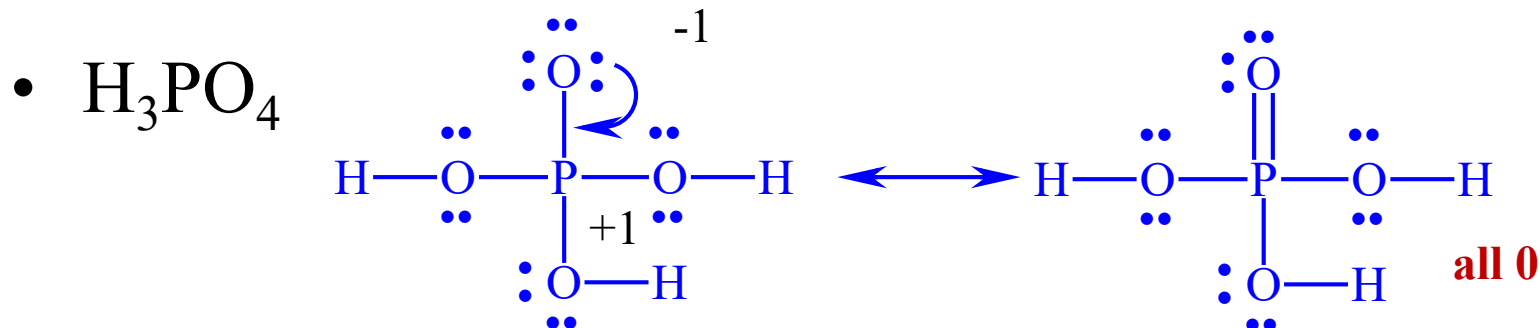
# Practice - Identify Structures with Better or Equal Resonance Forms and Draw Them



none



# Practice - Identify Structures with Better or Equal Resonance Forms and Draw Them

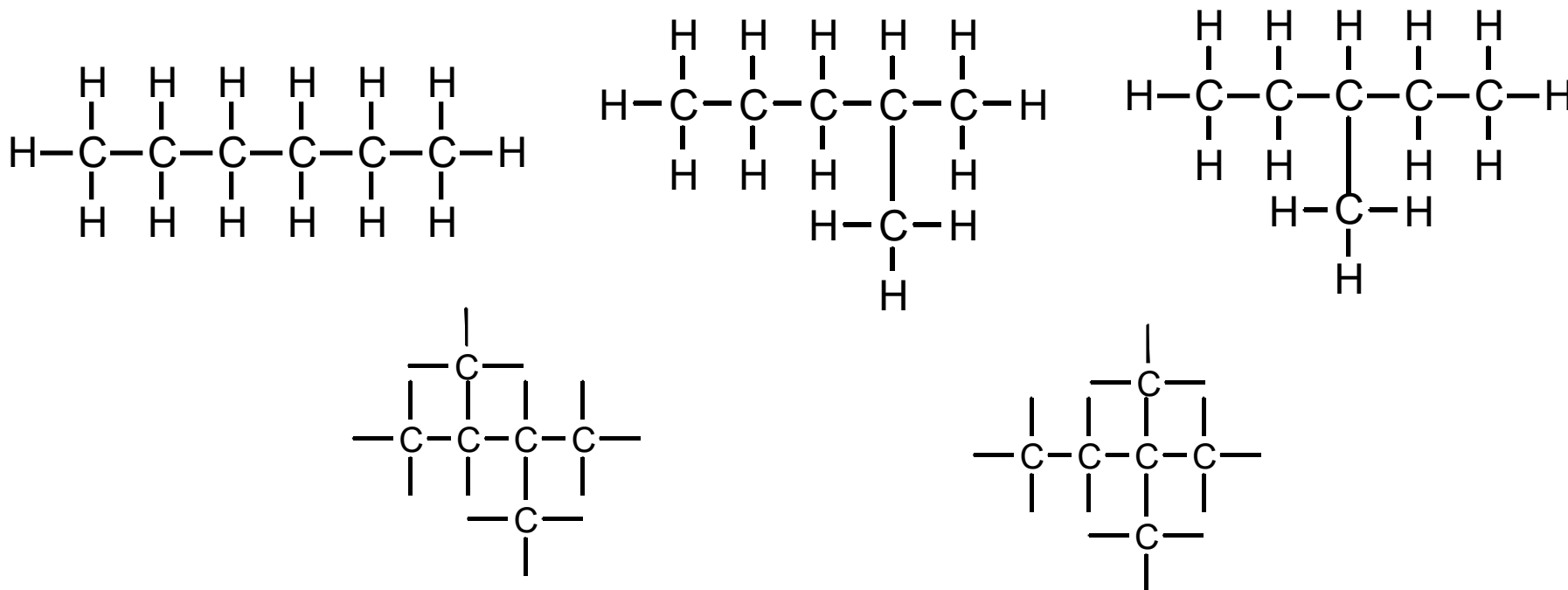


none

# ISOMERS & Coordinate Covalent Bonds:

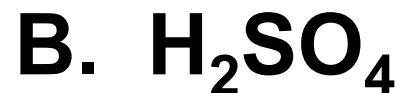
Structural isomers are compounds that possess the same chemical formula but different connectivity among the various atoms. For example, consider the formula  $C_2H_6O$ , which can be written in two different ways: (1)  $CH_3CH_2OH$  or (2)  $CH_3OCH_3$ :

Draw the various structural isomers for the hexane  $C_6H_{14}$  molecule:



## LECTURE Problems on Lewis structure REVIEW:

Draw *the best possible* Lewis dot structures for each of the following compounds or ions shown below, and include resonance where appropriate:



## Activity in canvas



# Bond Enthalpies and Enthalpy of Reaction

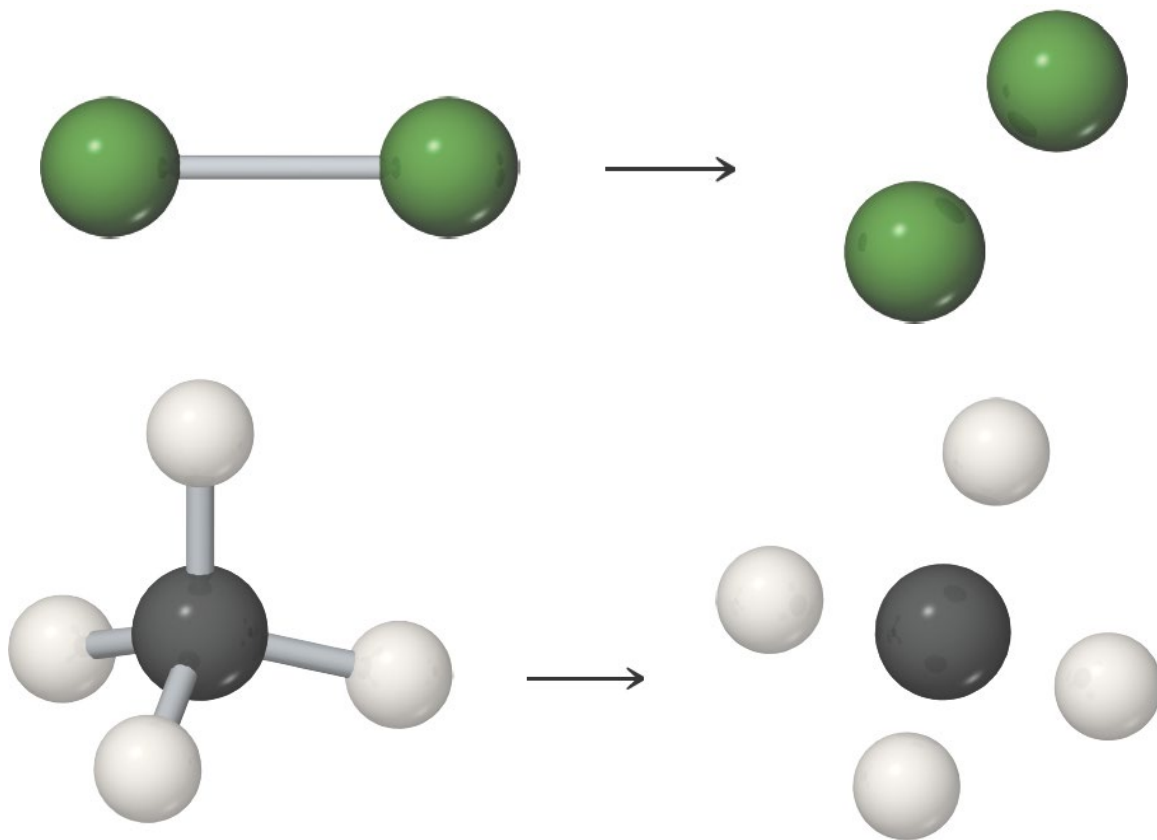
- **Add** bond energy for **all** bonds made (+)
- **Subtract** bond energy for **all** bonds broken (–)
- The result is an estimate of  $\Delta H$ .

$$\Delta H_{\text{rxn}} = \sum \left( \begin{array}{l} \text{bond enthalpies} \\ \text{of bonds broken} \end{array} \right) - \sum \left( \begin{array}{l} \text{bond enthalpies} \\ \text{of bonds formed} \end{array} \right)$$



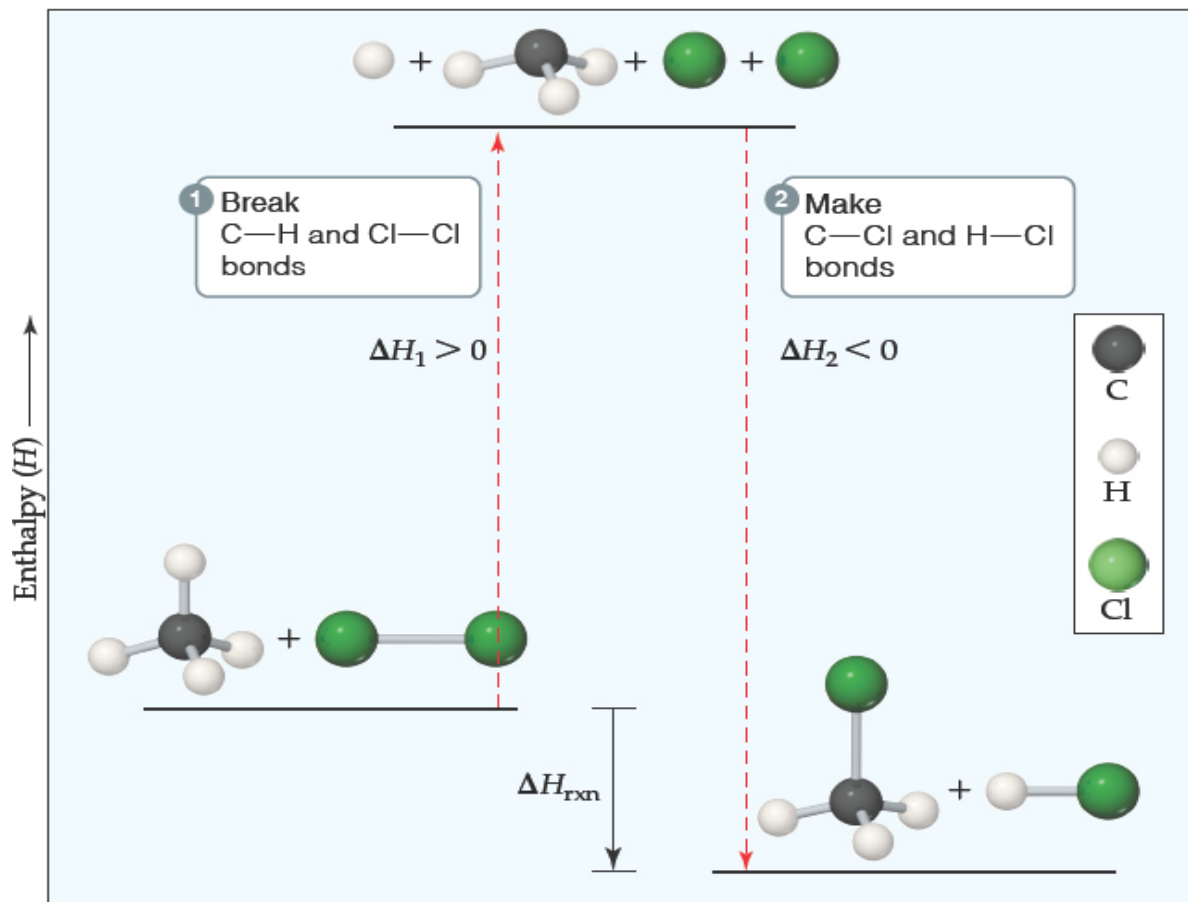
# Bond Enthalpy

The enthalpy associated with breaking one mole of a particular bond in a gaseous substance.



# Bond Enthalpies and Enthalpy of Reaction

So, we can predict whether a chemical reaction will be endothermic or exothermic using bond energies.



## Bond Energies (Enthalpies) BDE

$$\Delta H^\circ = \Sigma BE \text{ (bonds broken)} - \Sigma BE \text{ (bonds made)}$$

- A. All bond enthalpies listed in your textbook are **POSITIVE** because heat must be supplied to break a bond.
- B. Therefore, bond breaking is always **ENDOTHERMIC**, and bond formations is always **EXOTHERMIC**.
- C. Assume that the average bond energy applies regardless of the specific molecular environment; intermolecular interactions are expected to be minimal and hence are **NOT** taken into account.
- D. These calculations are limited to cases where **ALL** reactants/products are in the gas phase!

# Average Bond Enthalpies- revisited

- Bond enthalpies are positive, because bond breaking is an endothermic process.
- These are **averages** over many compounds; not every bond for a pair of atoms has the same bond energy.

**Table 8.3** Average Bond Enthalpies (kJ/mol)

Single Bonds							
C-H	413	N-H	391	O-H	463	F-F	155
C-C	348	N-N	163	O—O	146		
C-N	293	N-O	201	O-F	190	Cl-F	253
C-O	358	N-F	272	O-Cl	203	Cl-Cl	242
C-F	485	N-Cl	200	O-I	234		
C-Cl	328	N-Br	243			Br-F	237
C-Br	276			S-H	339	Br-Cl	218
C-I	240	H-H	436	S-F	327	Br-Br	193

# Average Bond Enthalpies

<b>Single Bonds</b>							
C-S	259	H-F	567	S-Cl	253		
		H-Cl	431	S-Br	218	I-Cl	208
Si-H	323	H-Br	366	S-S	266	I-Br	175
Si-Si	226	H-I	299			I-I	151
Si-C	301						
Si-O	368						
Si-Cl	464						
<b>Multiple Bonds</b>							
C=C	614	N=N	418	O=O	495		
C,C	839	N,N	941				
C=N	615	N=O	607	S=O	523		
C,N	891			S=S	418		
C=O	799						
C,O	1072						

# Estimate the Enthalpy of the Following Reaction



reaction involves breaking 1 mol H-H and 1 mol O=O  
and making 2 mol H-O and 1 mol O-O

bonds broken (energy cost)

$$(+436 \text{ kJ}) + (+498 \text{ kJ}) = +934 \text{ kJ}$$

bonds made (energy release)

$$2(464 \text{ kJ}) + (142 \text{ kJ}) = -1070$$

$$\Delta H_{\text{rxn}} = (+934 \text{ kJ}) + (-1070. \text{ kJ}) = -136 \text{ kJ}$$

(Appendix  $\Delta H^\circ_{\text{f}} = -136.3 \text{ kJ/mol}$ )

## Examples on Bond Energy

**Problem #1:** Estimate the enthalpy change of the reaction between gaseous iodoethane and water vapor:



<i>Bond Energies (kJ/mol):</i>	<i>C-O</i>	<i>360</i>	<i>H-O</i>	<i>463</i>
	<i>C-I</i>	<i>238</i>	<i>H-I</i>	<i>299</i>

## ACTIVITY on Bond Energy

**Problem #2:** Estimate the standard enthalpy of the following reaction:



<i>Bond Energies (kJ/mol):</i>	<i>C-F</i>	<i>485</i>	<i>C-Cl</i>	<i>339</i>
	<i>H-F</i>	<i>565</i>	<i>H-Cl</i>	<i>431</i>



# Average Bond Enthalpies- revisited

- Bond enthalpies are positive, because bond breaking is an endothermic process.
- These are **averages** over many compounds; not every bond for a pair of atoms has the same bond energy.

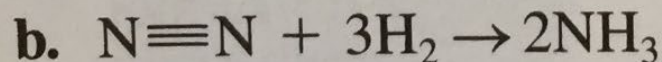
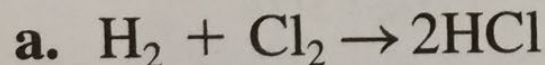
**Table 8.3** Average Bond Enthalpies (kJ/mol)

Single Bonds		C≡N	891				
C-H	413	N-H	391	O-H	463	F-F	155
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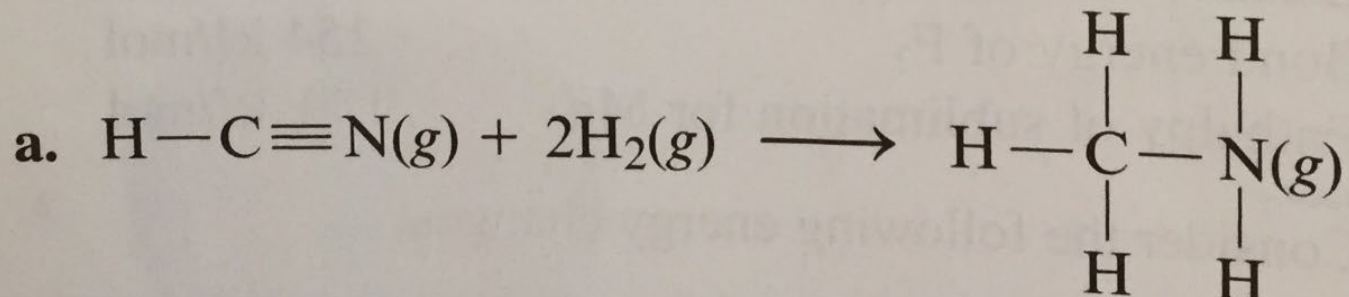
# Extra questions

## Bond Energies

**65.** Use bond energy values (Table 8.4) to estimate  $\Delta H$  for each of the following reactions in the gas phase.



**66.** Use bond energy values (Table 8.4) to estimate  $\Delta H$  for each of the following reactions.



*H-Cl*    431

*H-H*    436

*C l-C l*    242

# VSEPR MODEL

## Valence Shell Electron Pair Repulsion Model

A model for predicting the shapes of molecules and ions in which valence shell electron pairs are arranged about each atom so that electron pair repulsion is minimized. VSEPR states that electron pairs repel one another, whether they are in chemical bonds (bonding pairs) or unshared (lone pairs). Electron pairs assume orientations about an atom to minimize repulsions.

## ELECTRONIC GEOMETRY

The general shape of a molecule determined by the number of electron pairs around the central atom occupying different quadrants. Gives starting point for bond angle.

## MOLECULAR GEOMETRY

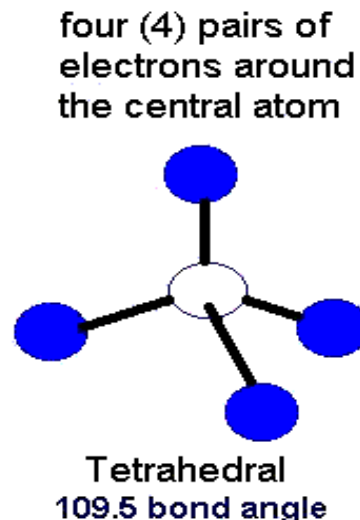
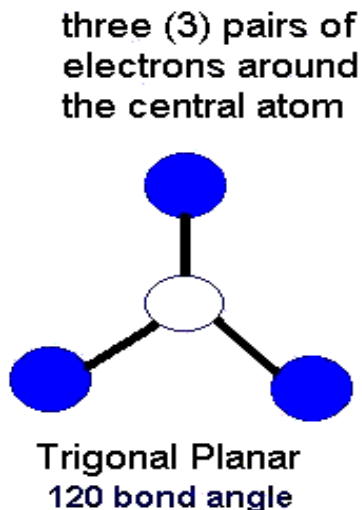
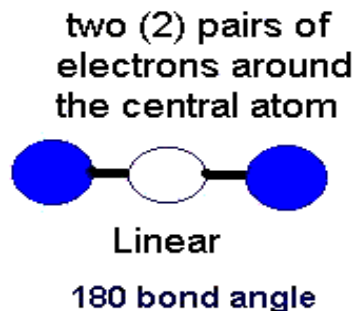
The general shape of a molecule determined by the relative positions of the atomic nuclei. The nonbonding electron pairs modify the geometry.

# VSEPR MODEL

I. Draw the Lewis dot structure.

II. Determine the **electronic geometry** by counting the number of pairs of electrons around the central atom occupying different quadrants (top, bottom, left, right). This geometry gives the initial bond angle.

<u>Pairs of e-</u>	<u>geometry</u>	<u>bond angle</u>
2	linear	180°
3	trigonal planar	120°
4	tetrahedral	109.5°
5	trigonal bipyramidal	120° & 90°
6	octahedral	90°



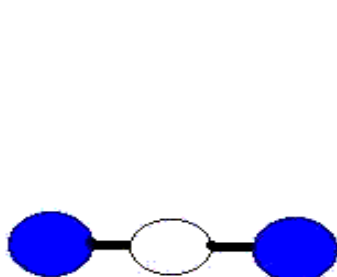
The structure for the first three geometries is given in these notes, the other two can be found in your textbook.

# VSEPR MODEL

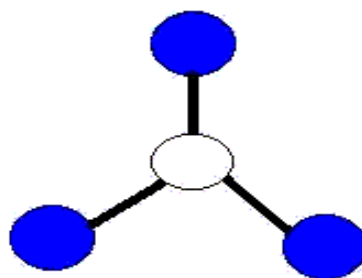
III. Next, using the electronic geometry, determine the number of bonding and nonbonding electron pairs then arrange the electron pairs as far apart as possible.

- nonbonding pairs require more space than bonding pairs.
- multiple bonds require more space than single bonds.

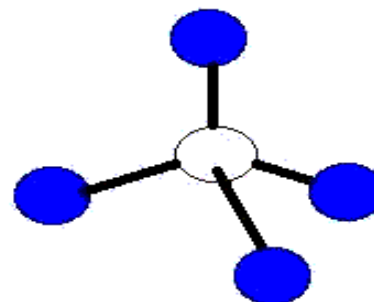
IV. The direction in space of the bonding pairs give the **molecular geometry** modified by the position of the nonbonding pairs.



Linear

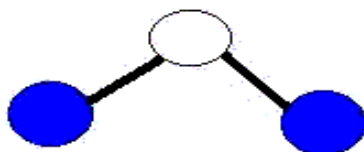


Trigonal Planar

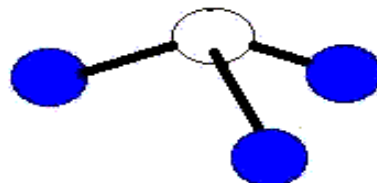


Tetrahedral

Bent or Angular



Trigonal Pyramidal



# Table describing Molecular Geometry

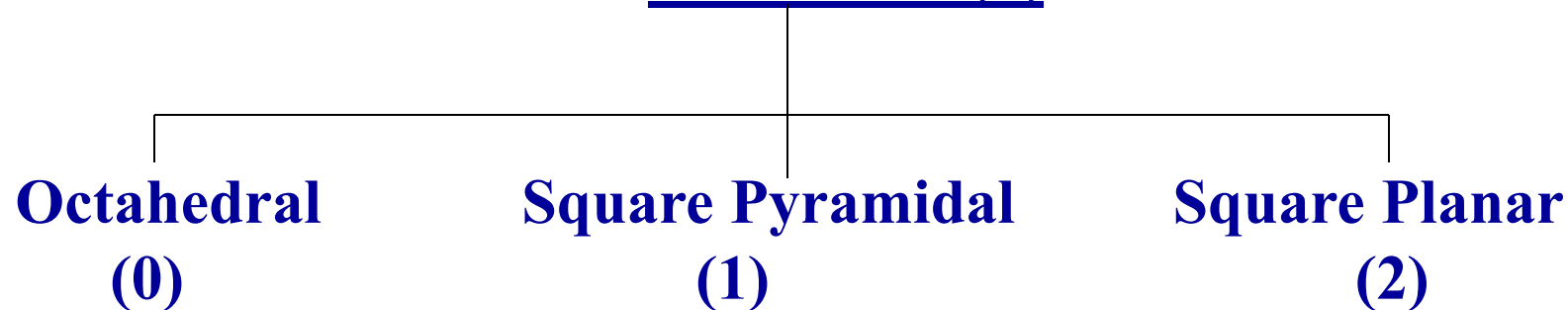
## VSPER Theory

Number of e- pairs	electronic geometry	bonding e- pairs	nonbonding e- pairs	molecular geometry
<b>2</b>	<b>linear</b>	<b>2</b>	<b>0</b>	<b>linear</b>
<b>3</b>	<b>trigonal planar</b>	<b>3</b>	<b>0</b>	<b>trigonal planar</b>
<b>3</b>	<b>trigonal planar</b>	<b>2</b>	<b>1</b>	<b>bent</b>
<b>4</b>	<b>tetrahedral</b>	<b>4</b>	<b>0</b>	<b>tetrahedral</b>
<b>4</b>	<b>tetrahdral</b>	<b>3</b>	<b>1</b>	<b>trigonal pyramidal</b>
<b>4</b>	<b>tetrahedral</b>	<b>2</b>	<b>2</b>	<b>bent</b>

## Trigonal Bipyramidal (5)



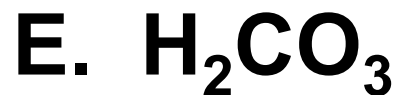
## Octahedral (6)



The above flow chart summarizes the relationship between the electronic to molecular geometries for trigonal bipyramidal & octahedral. The number in parenthesis denotes the number of nonbonding pairs of electrons.

## LECTURE Problems on Lewis structure

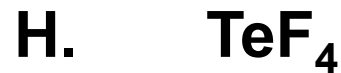
Draw *the best possible* Lewis dot & VSEPR structures for each of the following compounds or ions shown below, and include resonance where appropriate, describe polarity:





## Lecture Examples on Lewis structure & VSEPR:

Draw the best possible Lewis dot structures incorporating VSEPR model for each of the following compounds or ions shown below, and include resonance hybrids or isomers where appropriate:



More  
examples  
in canvas

# POLARITY OF MOLECULES

Molecules can also be described as either polar or nonpolar.

When the individual dipole moments associated with each bond in the molecule cancel out due to symmetry or if no dipole moment exist, the molecule can be classified as a **nonpolar molecule**. Nonpolar molecules have no overall dipole moment. Otherwise, if an overall dipole moment exist, the molecule is **polar**.

## Lecture Examples on Lewis structure & VSEPR:

Draw the best possible Lewis dot structures incorporating VSEPR model for each of the following compounds or ions shown below, and include resonance hybrids or isomers where appropriate: POLARITY

