# Molecular Structure

**1. Determine Lewis structure.**

**2. Use VSEPR to determine electron pair geometry.**
**(count electron domains: double and triple bonds counted as one domain!).**

**3. Use electron pair geometry to determine hybrid orbitals.**

**4. Determine molecular geometry. Focus on <u>bonded-electron pairs</u> ONLY to determine the molecular geometry (MG)**

**5. Is the molecule polar?**
**To answer this, use knowledge of:**

- **Molecular shape**
- **Bond Polarity**

**To determine the polarity of a molecule that has more than 2 atoms:**

**a) find molecular shape (3D)**
**b) find "bond" dipoles (using electronegativity differences)**
**c) use vector "analysis" to find net molecular dipole**

Lecture 7

## Shape, Polarity, Hybrid Orbitals

Draw Lewis structures for the following molecules. Determine the electron pair geometry and the molecular geometry for each. (Draw pictures if you want but be sure to include the **name** of the geometries.) What hybrid orbitals are used in bonding? Which of these molecules are polar?

| Molecular formula | Lewis structure | $e^-$ pair geometry | Molecular geometry | polar? yes/no | Hybrid orbitals |
|---|---|---|---|---|---|
| $NF_3$ | | | | | |
| $BF_3$ | | | | | |
| $ClF_3$ | | | | | |
| $ClO_4^-$ | | | | | |
| $PF_5$ | | | | | |
| $BrF_5$ | | | | | |
| $CO_2$ | | | | | |
| $XeF_2$ | | | | | |
| $OF_2$ | | | | | |

| # of electron domains | # of atomic orbitals | Names of atomic orbitals | Names of hybrid orbitals |
|---|---|---|---|
| 2 | 2 | s+p | sp |
| 3 | 3 | s+p+p | $sp^2$ |
| 4 | 4 | s+p+p+p | $sp^3$ |
| 5 | 5 | d+s+p+p+p | $dsp^3$ |
| 6 | 6 | d+d+s+p+p+p | $d^2sp^3$ |

## Sample Problem

Indicate the hybrid orbitals used by the central atom in each of the following molecules.

(A) $BCl_3$

(B) $BeBr_2$

(C) $XeO_3$

(D) $ClF_3$

(E) What hybrid orbitals are used by the two oxygen atoms in acetic acid? ($CH_3COOH$) ***Note:*** Each O may have a different hybridization.

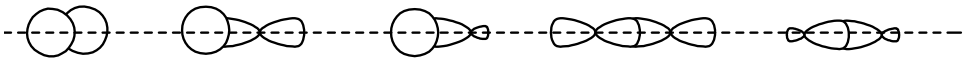
**Covalent bonding: overlap of (two singly occupied) atomic orbitals to form a new (doubly occupied molecular) orbital, allowing for sharing of electrons by the two nuclei.**

## Bond Types

### σ-bond

- **results from head-on overlap of orbitals**
- **electron density is symmetric about the internuclear axis: between nuclei.**

**Examples:**

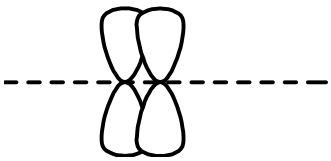


***s-s*** ***s-p*** ***s-sp$^x$*** ***p-p*** ***sp$^x$-sp$^y$***

**where sp$^x$ and sp$^y$ are hybrids orbitals**

### π-bond

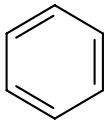
- **results from sideways overlap of orbitals**
- **electron density is above and below the internuclear axis.**



**Sample Problem**

How many σ and π bonds are in the following molecule? *(Hint: Draw out the <u>complete</u> Lewis structure before counting.)*

$CH_3COOH$



## Summary of Covalent bonding

1. **Draw Lewis Structure**

2. **Use VSEPR to determine shape**
   - **e- pair geometry**
   - **molecular geometry**

3. **What hybrid orbitals are involved in bonding?**
   **Determined by electron pair geometry.**
   **(Know the shapes of the hybrid orbitals.)**

4. **Is the molecule polar?**
   **Determined by molecular geometry.**

**Remember:**

- **Each single bond = covalent bond**
  **= σ bond**

- **A covalent bond forms when orbitals overlap.**
  **σ-bond: head-on overlap**
  **π-bond: sidewise overlap**

**Group Problems** **Name _____**

**Hybrid Orbitals, Bonding**

1. Using the following structure: $H_2C=C=CH_2$

a) How many sigma bonds are there? How many pi bonds?

b) What is the hybridization of the central C atom?

(a) sp
(b) $sp^2$
(c) $sp^3$
(d) $dsp^3$
(e) $d^2sp^3$

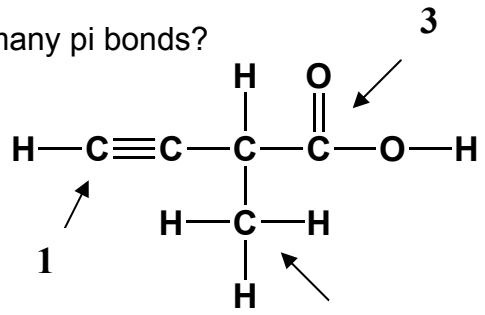
c) What is the hybridization of the terminal carbon atoms?

d) What is the C=C=C bond angle? What is the H—C—H bond angle?

a) 90°
b) 109.5°
c) 120°
d) 180°

2. Using the following structure:

a) How many sigma bonds are there? How many pi bonds?

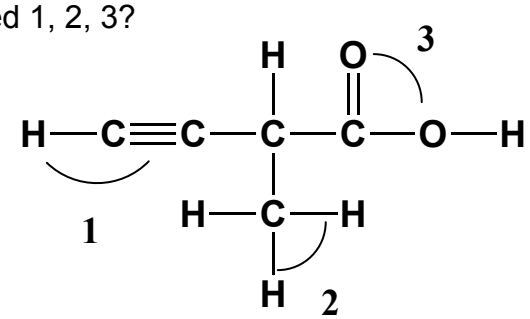



b) What is the hybridization of the two O atoms?

(a) sp
(b) $sp^2$
(c) $sp^3$
(d) $dsp^3$
(e) $d^2sp^3$

c) What is the hybridization of the carbon atoms labeled 1, 2 and 3?

d) What are the angles of the bonds labeled 1, 2, 3?




a) 90° c) 120°
b) 109.5° d) 180°

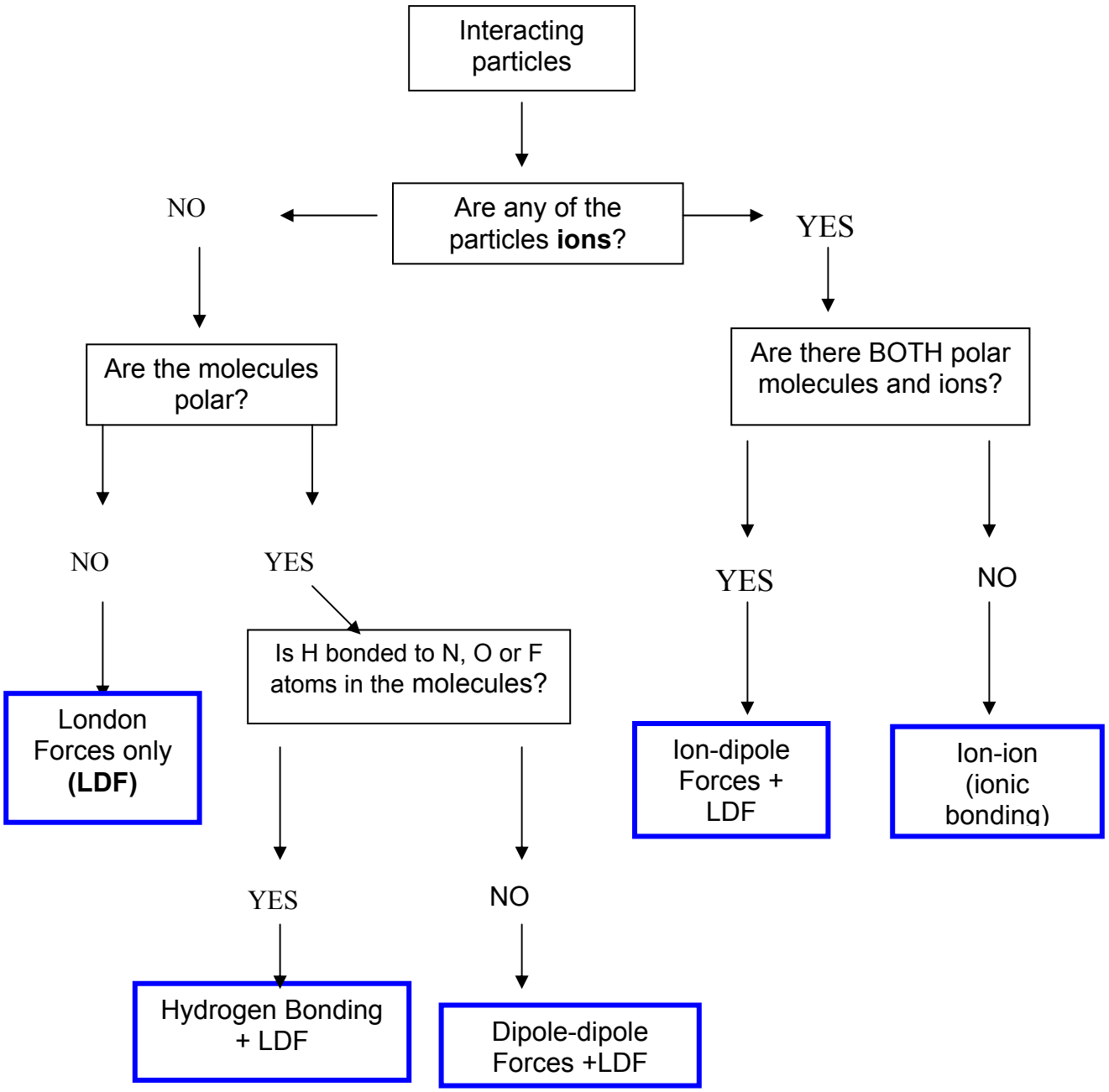
**Strength of IM forces depends on:**

- **Q** — **charge on ion**
- $\mu$ — **dipole moment**
- $\alpha$ — **polarizability**

**$\alpha$ - polarizability: ease with which electrons clouds become distorted**
**$\alpha$ increases as number of electrons increases**
**$\alpha$ increases as size (MW) increases**

| TYPES OF INTERMOLECULAR FORCES | Depends on |
|---|---|
| **Ion-Ion**<br>**ionic bond** | **Q** |
| **Ion-Dipole**<br>**Ions in aqueous solutions of electrolytes** | **Q, $\mu$** |
| **Dipole-Dipole** | **$\mu$** |
| **Ion-Induced Dipole**<br>**ions in nonpolar solvents** | **Q, $\alpha$** |
| **Dipole-Induced Dipole**<br>**polar molecules in nonpolar solvents** | **$\mu$, $\alpha$** |
| **Dispersion**<br>**induced-dipole induced dipole** | **$\alpha$** |
| **Hydrogen Bonding**<br>**must have H bonded to N,O,F** | **directional dipole-dipole** |

# Flow Chart For Determining Intermolecular Forces




Note: LDF = London Dispersion Forces
All molecules have LDF in addition to other intermolecular forces.

## Sample Problem

What type (or types) of intermolecular forces would be important in the following molecules or atoms? *(It is possible for a molecule to interact via more than one of these. List **ALL** that are important.)* To answer this question you should:

1. Draw Lewis Structures and determine the shape and polarity of each molecule.
2. Use the flowchart on page 37 of the Study Guide to determine the important intermolecular forces.

| | Lewis Structure | Important Intermolecular forces |
|---|---|---|
| **HCl** | | |
| **Ar** | | |
| **HF** | | |
| **$CO_2$** | | |
| **$SO_2$** | | |
| **$CH_4$** | | |
| **NO** | | |
| **$H_2S$** | | |

**Group Problems** **Name _____**
**Intermolecular Forces**

1. Which one of the following molecules has the highest normal boiling point?

(a) $CH_3Cl$
(b) $CH_3Br$
(c) $CH_3I$
(d) $CH_4$
(e) $CH_3OH$

HINT: Use the flow chart on 34 of the Study guide to help you determine the important intermolecular forces of each molecule.

Rank the molecules listed above from lowest normal boiling point to highest normal boiling point.

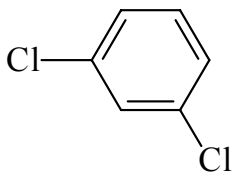
2. Which intermolecular forces are important for the pure liquid $CH_3F$?

A. London forces only
B. dipole-dipole interactions only
C. H-bonding only
D. London forces and dipole-dipole interactions
E. London forces, H-bonding and dipole-dipole interactions

3. What type (or types) of intermolecular forces would be important in the following molecules or atoms? *(It is possible for a molecule to interact via more than one of these. List **ALL** that are important.)*

Choose from these answers:
**a)** London Dispersion Forces **b)** dipole-dipole **c)** H-bonding, **d)** ion-ion (lattice energy)

i)

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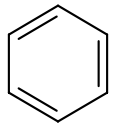
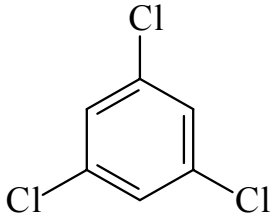


iii)




iv)