CHAPTER 8

Molecular Structure & Covalent Bonding Theories

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Molecular Shapes and Bonding

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7. Tetrahedral Electronic Geometry: AB_4
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9. Tetrahedral Electronic Geometry: AB_2U_2
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12. Octahedral Geometry
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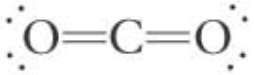
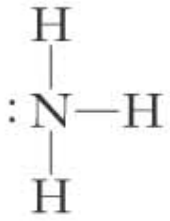
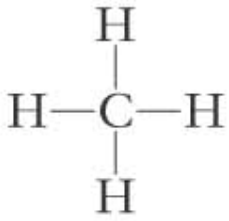
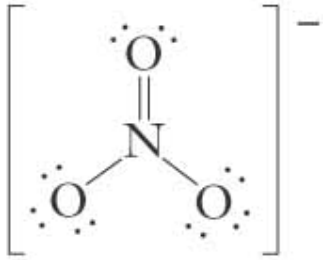
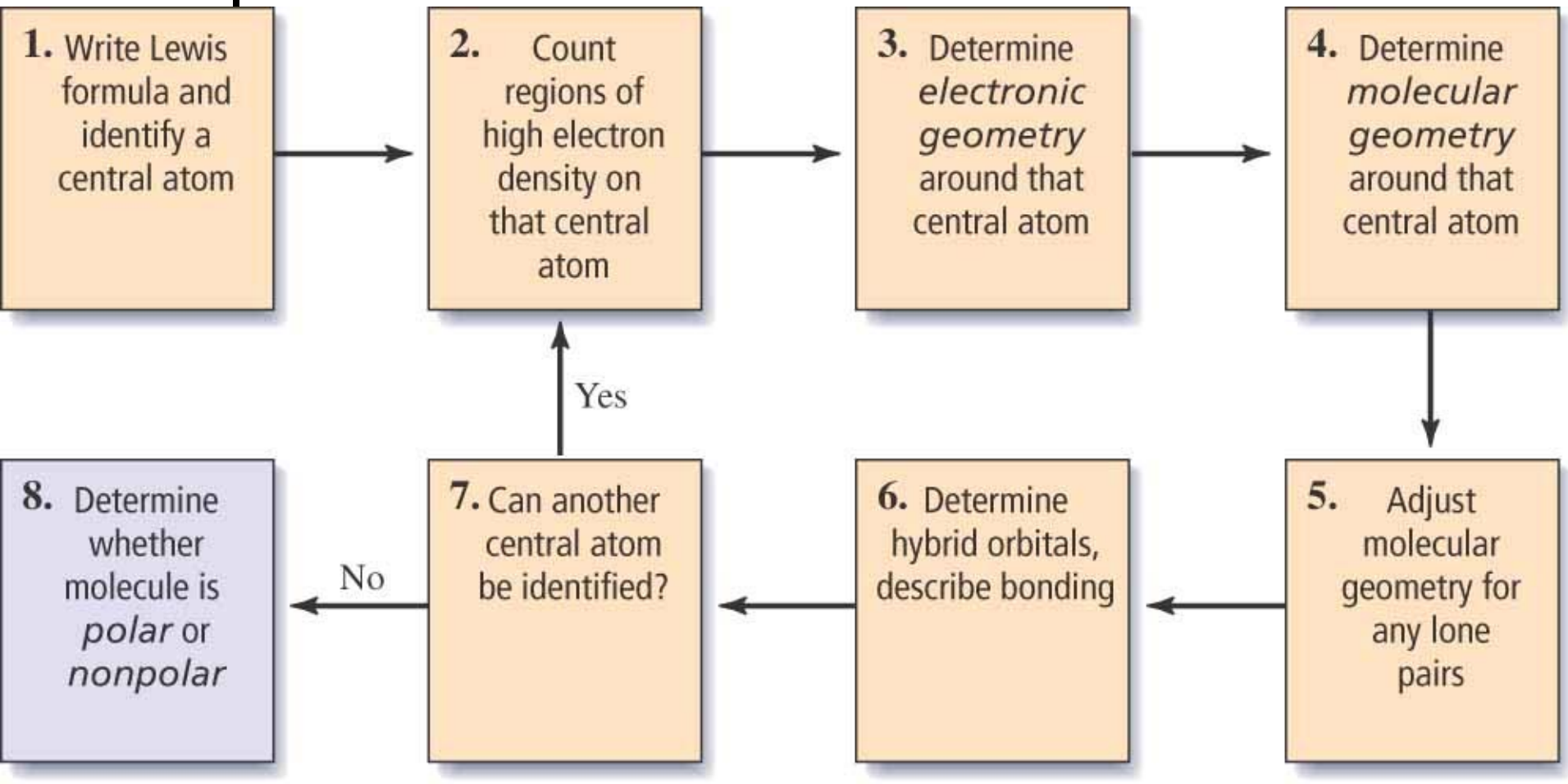
14. Compounds Containing Triple Bonds

Two Simple Theories of Covalent Bonding

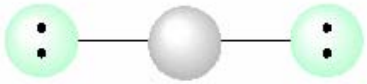
- **Valence Shell Electron Pair Repulsion Theory (VSEPR)**
  - **R. J. Gillespie in the 1950's**
- **Valence Bond Theory**
  - **Involves the use of hybridized atomic orbitals**
    - **L. Pauling in the 1930's & 40's**

Formula:	CO_2	NH_3	CH_4	NO_3^-
Lewis dot formula:				
Central atom:	C	N	C	N
Number of atoms bonded to *central atom:*	2	3	4	3
Number of unshared pairs on *central atom:*	0	1	0	0
Total number of regions of high electron density on *central atom:*	2	4	4	3

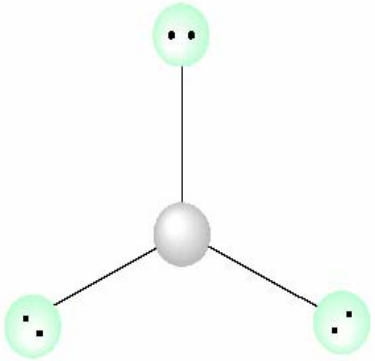


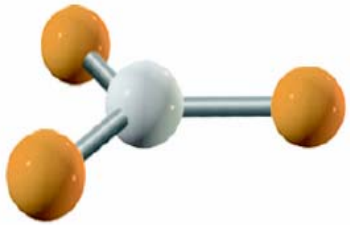
VSEPR Theory

linear;
180°

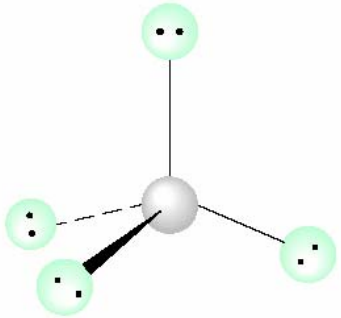


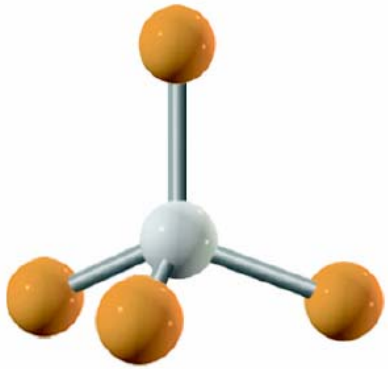
trigonal planar;
120°



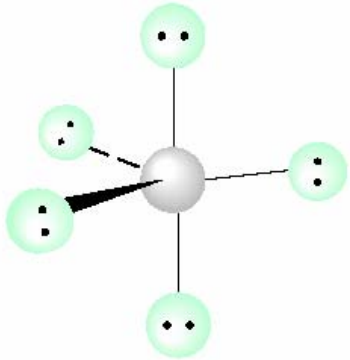


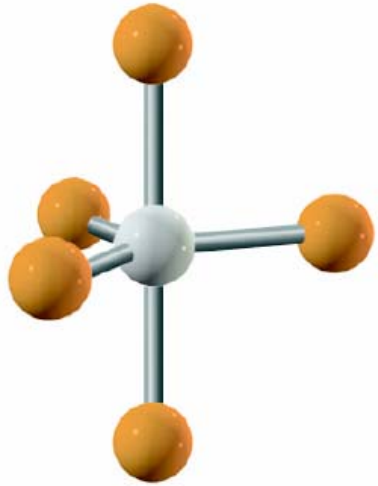
tetrahedral;
109.5°



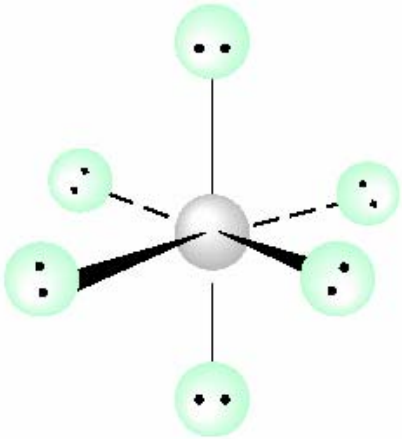


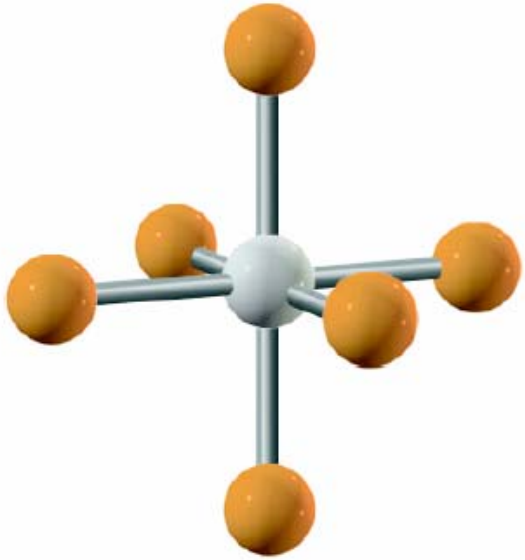
trigonal bipyramidal;
90°, 120°, 180°





octahedral;
90°, 180°





VSEPR Theory

- Frequently, we will describe two geometries for each molecule.

1. ***Electronic geometry*** is determined by the locations of regions of high electron density around the central atom(s).
2. ***Molecular geometry*** determined by the arrangement of atoms around the central atom(s).

Electron pairs are not used in the molecular geometry determination just the positions of the atoms in the molecule are used.

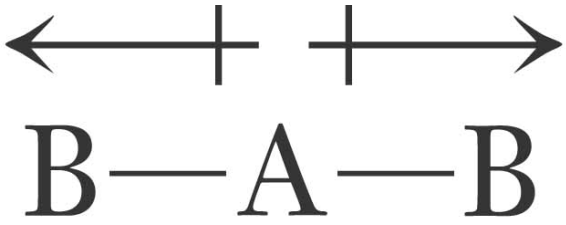
VSEPR Theory

- Lone pairs of electrons (unshared pairs) require more volume than shared pairs (bonding pairs).
- Repulsion strengths

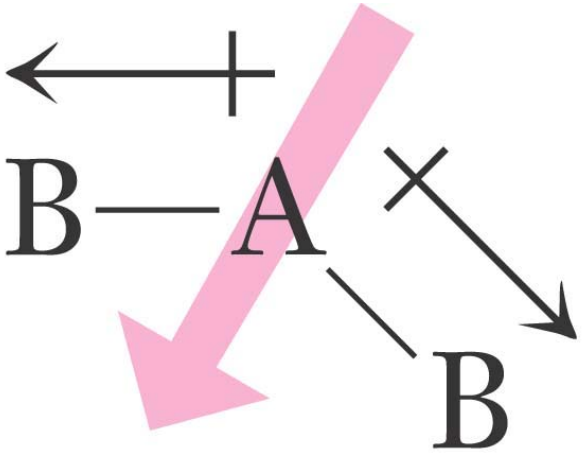
  lp/lp > lp/bp > bp/bp

Polar Molecules: The Influence of Molecular Geometry

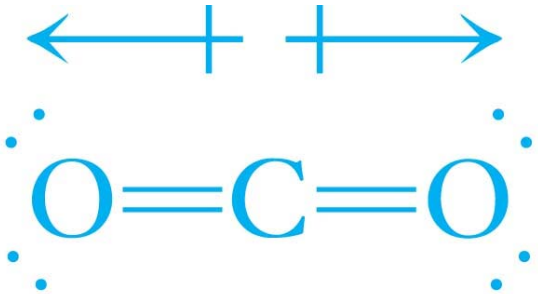
- Molecular geometry affects molecular polarity.
  - Due to the effect of the bond dipoles and how they either cancel or reinforce each other.



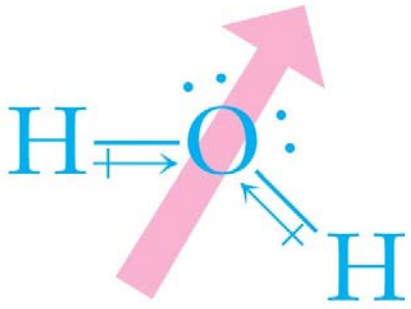
net dipole = 0
(nonpolar molecule)



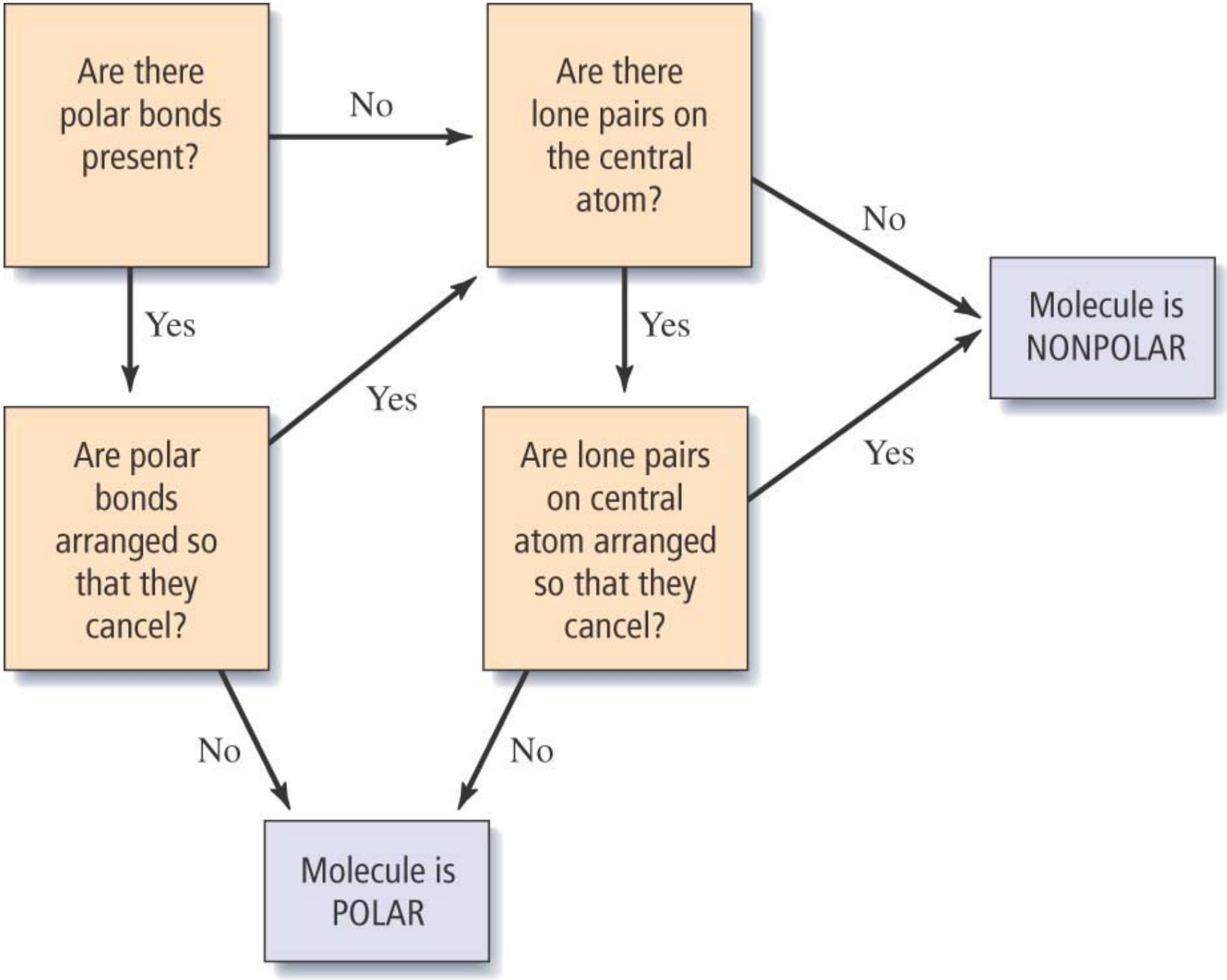
net dipole > 0
(polar molecule)



linear molecule;
bond dipoles cancel;
molecule is nonpolar



angular molecule;
bond dipoles do not cancel;
molecule is polar



Valence Bond (VB) Theory

- Covalent bonds are formed by the **overlap** of atomic orbitals.
- Atomic orbitals on the central atom can mix and exchange their character with other atoms in a molecule.
  - Process is called **hybridization**.

Molecular Shapes and Bonding

- In the next sections we will use the following terminology:

  A = central atom

  B = bonding pairs around central atom

  U = lone pairs around central atom

- For example:

  AB_3U designates that there are **3 bonding pairs** and **1 lone pair** around the central atom.