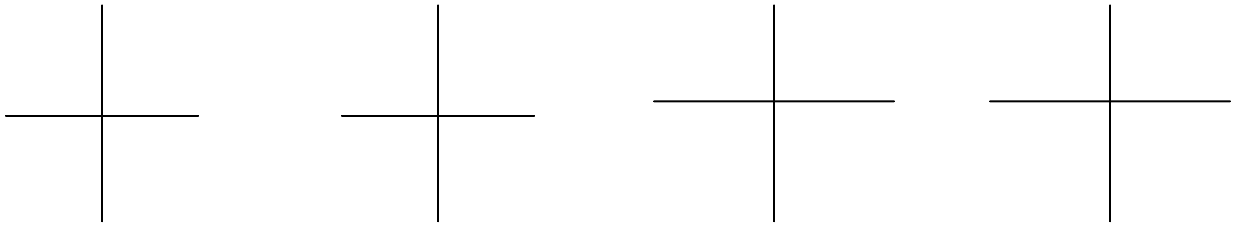
# *Chapter 1. Structure and Bonding*

## Atomic Structure

Quantum Mechanics tells us that electrons in atoms exist in allowed energy states called ____________ _____________.



Notice the ____________ in the 2p orbitals:

***Three rules*** for determining the ________________ ______________ electron configuration:

1.

2.

3.

Give the ground state electron configurations of:

H

C

Br

***Three different models are used to explain why atoms form bonds.***

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***Bonding Model Number 1:***

*The octet rule:*

Three examples:

$H_2$

NaCl

$CH_4$

*Important Learning Objective:* Be able to draw the complete Lewis Structure of any compound.

Shortcut: It is easy to predict the number of bonds that an atom of a particular element can form:

**Examples**: Draw the Lewis Structure (also called “Kekulé Structure” or “Line-Bond Structure”) of these compounds:

| **compound** | **Lewis Structure** | **Condensed Structural Formula** |
|---|---|---|
| $C_2H_6$ | | |
| $CH_5N$ | | |
| $CH_4O$ | | |
| $C_2H_4$ | | |
| $C_2H_2$ | | |
| $CH_2O$ | | |
| $C_2H_6O$ | | |

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***Bonding Model Number 2:***

Terms associated with VBT:

The main idea behind _______________ _______________ _________________:

Examples: H + H → H–H

H + F → H–F

sigma bond ($\sigma$ bond)

pi bond ($\pi$ bond)

1 single bond =

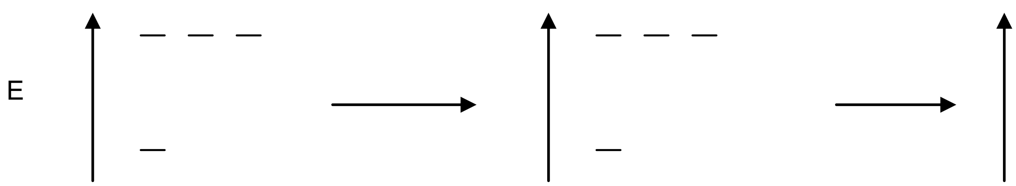
1 double bond =

1 triple bond =

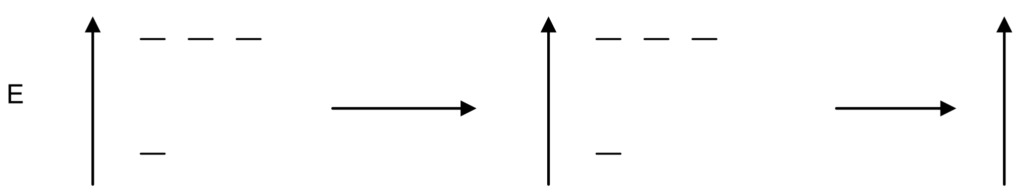
- Whenever simple atomic orbital overlap is inadequate to explain certain bond properties (such as equivalency of bonds, bond angles, etc.) the concept of ________________________ is invoked.
- The process of ____________________ corresponds to a mixing of orbitals (an imaginary process accomplished mathematically) resulting in new orbitals called ___________________ _________________.

***Thought experiment***: Give electron configuration of a ground state C atom.

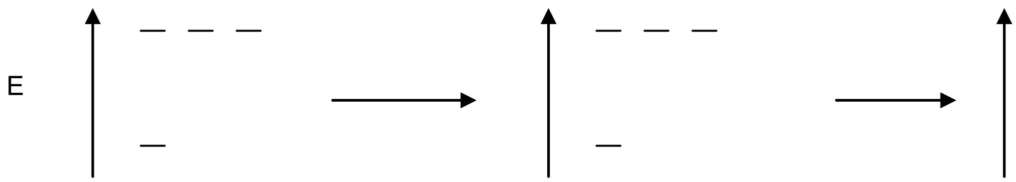
$sp^3$ hybridization:




$sp^2$ hybridization:



sp hybridization:




***Be able to determine the hybridization of any atom in a molecule.***

Count the number of

plus the number of

If # σ bonds + # lone pairs = 2, then

If # σ bonds + # lone pairs = 3, then

If # σ bonds + # lone pairs = 4, then

Example: Determine the hybridization of every non-hydrogen atom in each molecule below:

$CH_2$=$CHCH_3$ $NH_3$ $H_2O$ HCHO $CH_3OH$ $C_2H_2$

***Key point in Valence Bond Theory: The better the ______________, the ________________ the bond.***

***There are two ways to quantitatively describe the strength of a covalent bond:***

1.

2.

**Bond Dissociation Energy (D):**

example: $H_2$

Important: Bond Breaking is always ______________________ (or ____________________________)

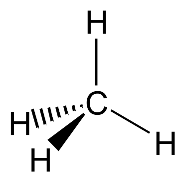
Bond Formation is always _____________________ (or ____________________________)

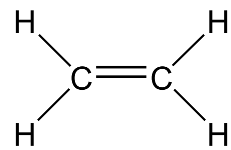
**Bond Length:** C–C C=C C≡C

*Question*: Why isn't a double bond twice as strong as a single bond?

Why isn't a triple bond three times as strong as a single bond?

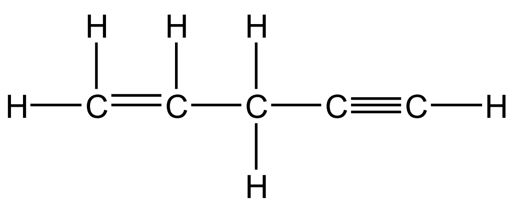
*Compare* the C–H bond lengths and bond strengths in these molecules:





*Example*: In the molecule below, determine:

a) the hybridization of each C atom
b) the relative strength and bond length of each C–C bond
c) the relative strength and length of each C–H bond



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***Bonding Model Number 3:***

1. Summary of Molecular Orbital (MO) Theory:

- Quantum Mechanics says :

  Electrons in ________________ exist in allowed energy states called ________________________________

  Electrons in ________________ exist in allowed energy states called ________________________________

- Think of MOs this way: they are formed from a ____________________________________________________

- Two important types of MOs:

- Determining MO electron configuration is analogous to determining AO electron configuration:

2. Atomic Orbitals (AOs) and Molecular Orbitals (MOs):

- Two equivalent AOs will interact to form 2 MOs:
- The Bonding MO is _________________ in energy than the AOs.
- The antibonding MO is _______________ in energy than the AOs, and it has a _________ between the two atoms.
- One way to understand this: AOs and MOs are wave functions (QM says $e^-$ have wave characteristics).

--Two AOs can overlap constructively (wave reinforcement) to form a ______________ MO.

--Or they can overlap destructively (wave cancellation) to form an _________________________ MO.

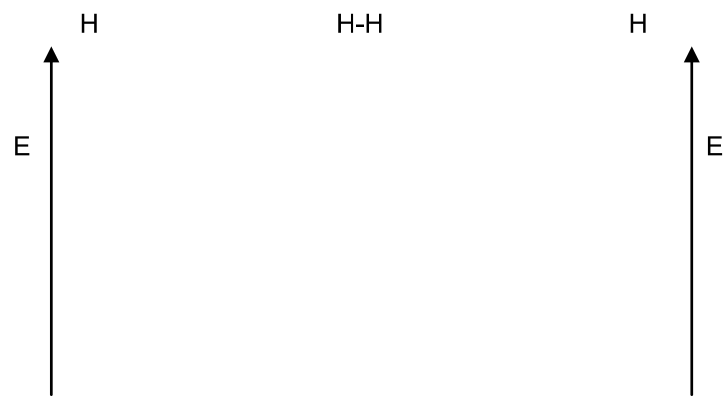
3. Bonding MOs are designated ______________and ___________ MOs.

Antibonding MOs are designated _____________ and ___________ MOs

(pronounced "sigma star" and "pi star" molecular orbitals).

4. When two equivalent s orbitals combine, they result in a _______ bonding MO and a __________ antibonding MO

**Example**: H + H → H-H




4. When two parallel p orbitals combine, they result in a _____ bonding MO and a _________ antibonding MO.


***Drawing Chemical Structures***

Be able to draw the condensed structure and skeletal structure of any organic compound.

Skeletal structures: 1) _____ and _____ atoms are usually not shown.

2) You should mentally supply sufficient hydrogen atoms by knowing that:

***Examples:***

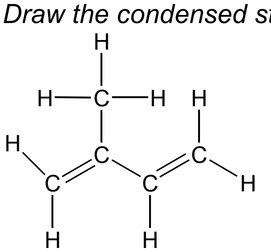
propane

pentane

2,3-dimethylpentane

cyclohexane

*Draw the condensed structure and the skeletal structure of isoprene, given the following Lewis structure:*



*Show the reaction of 1-butene with bromine, using condensed structures and skeletal structures:*

***Two common mistakes to avoid:***

1. Don't give carbon ____________________________________________

2. Don't imagine carbons ________________________________________

*Draw the condensed structures and the skeletal structures of:*

*1-butanol* *1-bromopropane* *3-chloropropene*