Lecture 3

Topics

Recap on Valence Bond Theory
Molecular Orbital Theory
Drawing Chemical Structures
Isomers
  - constitutional isomers
  - stereoisomers
Representative Organic Compounds

Props/Visuals

Large structural models
  - cis/trans 2-butene (w/ π-orbital loops)
  - n-butane
  - iso-butane
V. Molecular Orbital Theory

A. Describes covalent bonding by using a mathematical combination of atomic orbitals (linear combination of atomic orbitals = LCAO's) on different atoms to form new molecular orbitals.

1. Additive combinations provide bonding MO's with an increase in e- density between the atoms.

2. Subtractive combinations provide antibonding MO's with a decrease in e- density between the atoms.

Example: dihydrogen $H_2$

\[ H_a \rightarrow H_b \]

\[ \Delta^* \text{antibonding} \rightarrow (H_a 1s - H_b 1s) \]

\[ H_a 1s \rightarrow l_s H_b \]

\[ \sigma^\text{bonding} \rightarrow \frac{1}{\sqrt{2}}(H_a 1s + H_b 1s) \]

3. Bond order is determined by $\# \text{bonding pairs} - \# \text{antibonding pairs}$.
B. Principles of MO Theory.
1. MO's are to molecules what AO's are to atoms - regions of space where electrons are most likely to be found.

2. MO's are formed by LCAO's and are equal in numbers to the AO's combined from the separate atoms.

3. Three types of MO's
   a. bonding MO's are lower in energy than the corresponding AO's and result in increased density between the bonded atoms.
   b. antibonding MO's are higher in energy than the corresponding AO's and result in decreased density between the atoms.
   c. non-bonding MO's are about the same energy as the corresponding AO's and result in no change in density between the atoms.

C. Advantages of MO Theory
   - it correctly predicts bonding interactions and molecular properties not correctly predicted by VB Theory.
VI. Drawing Chemical Structures

A. Lewis and Dash-bond structural formulas.

Example: Propane

\[
\text{H} - \text{C} - \text{C} - \text{C} - \text{H} \\
\text{H} \quad \text{H} \\
\text{H} \quad \text{H} \quad \text{H}
\]

B. Isomers:

Example: Butanes

\[
\text{H} - \text{C} - \text{C} - \text{C} - \text{H} \\
\text{H} \quad \text{H} \quad \text{H} \quad \text{H}
\]

\[
\text{H} - \text{C} - \text{C} - \text{C} - \text{H} \\
\text{H} \quad \text{H} \quad \text{H} \quad \text{H}
\]

B. Condensed Structural Formulas

\[
\text{CH}_3 \text{CH}_2 \text{CH}_2 \text{CH}_3
\]

\[
\text{CH}_3 \text{CH} \text{CH}_2 \text{CH}_3 \\
\text{CH}_3 \text{CH}_2 \text{CH} \text{CH}_3
\]
C. Bond Line Formulas

If heteroatom, must show it!

D. 3-D Formula Drawings.
VII. Introduction to Isomers

A. Isomers - compounds with same chemical formula, but different structures.

B. Constitutional isomers - different order of connection of atoms.

Example: pentane C\(_5\)H\(_{12}\)

\[ \text{Diagrams of constitutional isomers of pentane with different chlorine substitutions.} \]
C. Stereoisomers - same order of connection of atoms, but different geometries.

Example: 2-butene

\[
\begin{align*}
\text{trans} & \quad \text{cis} \\
\text{H} & \quad \text{H} \\
\text{H}_3\text{C} & \quad \text{H}_3\text{C} \\
\text{C} & \quad \text{C} \\
\text{C} & \quad \text{C} \\
\text{H}_3 & \quad \text{CH}_3 \\
\end{align*}
\]

Example: 1,3-Dichlorocyclopentane

\[
\begin{align*}
\text{trans} & \quad \text{cis} \\
\text{Cl} & \quad \text{Cl} \\
\text{Cl} & \quad \text{Cl} \\
\end{align*}
\]