Organic Chemistry II
CHEM 2211

Dr. Xiaodong Michael Shi
MW, 12:30 pm--01:45 pm
Atorvastatin (Lipitor): best selling drug in the world
(> $13 billion per year)
Topic I. Structure and Bonding

• Carbon
  ▪ Group #: 4A
  ▪ Atomic #: 6
  ▪ Element symbol: C
  ▪ Elemental name: carbon
  ▪ Atomic weight: 12.011
  ▪ Electron distribution: 1s\(^2\) 2s\(^2\)2p\(^2\)

• Carbon: the most important element to life!
  ▪ Blood: various minute by minute
  ▪ Bone: 0.8%
  ▪ Tissue: 67%
  ▪ Total amount in body: 16 kg
Topic I. Structure and Bonding

Only carbon forms strong single bond to itself that are stable enough to resist chemical attack under ambient conditions.
Topic I. Structure and Bonding

- **Bonding**: the joining of two atoms in stable arrangement.

  Lewis Structures

  Bond Length

  Bond Angle

  Geometry

  Formal Charge

  And ……..
Topic I. Structure and Bonding
Topic I. Structure and Bonding
Topic I. Structure and Bonding
Topic I. Structure and Bonding

- **Formal Charge**
  
  Knowing the following key 
  
  Valence electrons:
  
  Electron ownership:
Topic I. Structure and Bonding

- **Formal Charge**

  Knowing the following key #:

  - Valence electrons:

  - Electron ownership:

    Electron ownership: Unshared electrons + ½ of shared electrons

  Formal charge = # of valence electron – electron “owns”
Topic I. Structure and Bonding

- **Formal Charge**

\[
\begin{align*}
\text{Formal Charge of CH}_3
\end{align*}
\]

\[
\begin{align*}
\text{Formal Charge of CH}_2
\end{align*}
\]
Topic I. Structure and Bonding

- Formal Charge

\[\text{NO}_2\]
Topic I. Structure and Bonding

- **Octet rule**

\[
\begin{align*}
\text{H}_3\text{C} & \quad \text{Me} \\
\varepsilon &= 21
\end{align*}
\]

\[
\begin{align*}
\text{O} \\
\varepsilon &= 47
\end{align*}
\]
Degree of Unsaturation

\[ \text{DOU} = \frac{\sum (v-2) + 2}{2} = \frac{\#C \times 2 - \#H - \#X + \#N + 2}{2} \]

\( C_7H_{12}O_2 \)

\( C_6H_5NO_2 \)
Degree of Unsaturation

\[
\text{DOU} = \frac{\sum (v-2) + 2}{2} = \frac{\#C \times 2 - \#H - \#X + \#N + 2}{2}
\]

\[\text{C}_6\text{H}_5\text{NO}_2\]
Resonance: Re-allocation of electrons

- Single resonance structure does not represent the structure of a molecule, only the hybrid/combination does.

- Resonance structures are not in equilibrium. They are the different formats of a same molecule.

- Resonance structures are not isomers.
Topic I. Structure and Bonding

- Resonance: Re-allocation of electrons
### Topic I. Structure and Bonding

- **Bond length**
  - H-H: 0.74
  - H-F: 0.92
  - C-F: 1.33
  - C-H: 1.09
  - H-Cl: 1.27
  - C-Cl: 1.77
### Topic I. Structure and Bonding

#### Bond strength and bond length (C-C)

<table>
<thead>
<tr>
<th>Bond</th>
<th>length (Å)</th>
<th>strength (kcal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH$_3$-CH$_3$</td>
<td>1.53</td>
<td>88</td>
</tr>
<tr>
<td>CH$_2$=CH$_2$</td>
<td>1.34</td>
<td>152</td>
</tr>
<tr>
<td>CH≡CH</td>
<td>1.21</td>
<td>200</td>
</tr>
</tbody>
</table>
Topic I. Structure and Bonding

- Bond Angle
  - Linear $180^\circ$
  - Trigonal planar $120^\circ$
  - Tetrahedral $109.5^\circ$
Topic I. Structure and Bonding

- **Bond Angle**
  - Linear 180°
  - Trigonal planar 120°
  - Tetrahedral 109.5°
Topic I. Structure and Bonding

• Bond Angle
Topic I. Structure and Bonding

- Hybridization: SP3, SP2, SP

- $s$ factor
Topic I. Structure and Bonding

- Bond strength and bond length (C-H)

<table>
<thead>
<tr>
<th>Bond</th>
<th>length (Å)</th>
<th>strength (kcal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₃-H</td>
<td>1.11</td>
<td>98</td>
</tr>
<tr>
<td>CH₂=CH-H</td>
<td>1.10</td>
<td>104</td>
</tr>
<tr>
<td>CH≡C-H</td>
<td>1.09</td>
<td>125</td>
</tr>
</tbody>
</table>
Topic I. Structure and Bonding

• Electronic donating and Electron Withdrawing group

(EDG vs EWG)
Topic I. Structure and Bonding

- Electronic donating and Electron Withdrawing group
  
  (EDG vs EWG)
Topic II. Curved arrow electron pushing

- Curved arrow notation for electron moving
Topic II. Curved arrow electron pushing

• How to draw curved arrow notation:
  
  Where to start: pair of electrons

  Where to go: how or something can move
Topic II. Curved arrow electron pushing

- How to draw curved arrow notation: Where to start and where to go!
Topic II. Curved arrow electron pushing

- How to draw curved arrow notation: *Where to start and where to go!*
Topic II. Curved arrow electron pushing

• How to draw curved arrow notation: Where to start and where to go!
Topic II. Curved arrow electron pushing

- How to draw curved arrow notation: Where to start and where to go!
Topic II. Curved arrow electron pushing

- How to draw curved arrow notation: Where to start and where to go!

\[
\begin{align*}
\text{H} & \quad \text{C} \longrightarrow \text{C} \\
\text{C} & \quad \text{CH}_2
\end{align*}
\]
Topic II. Curved arrow electron pushing

- How to draw curved arrow notation: Where to start and where to go!
Topic III. Acid and Base Chemistry

- Acid/Base reaction

\[ \text{HA} \xleftrightarrow{\text{Keq}} \text{H}^+ + \text{A}^- \]
Topic III. Acid and Base Chemistry

- Acid/Base reaction

\[ \text{HA}_1 + \text{A}_2^- \xrightarrow{\text{Keq}} \text{HA}_2 + \text{A}_1^- \]
Q: What is the Keq? What is $\Delta G$?
Topic III. Acid and Base Chemistry

- Acid/Base reaction
Topic III. Acid and Base Chemistry

• Acid strength and pKa

Resonance effect and inductive effect

\[
\begin{align*}
&\text{H}_3\text{C-COOH} & &\text{HO} & &\text{H}_3\text{C-OH} \\
&\text{C} & &\text{OH} & &
\end{align*}
\]
Topic III. Acid and Base Chemistry

- Acid strength and pKa
Topic III. Acid and Base Chemistry

- Acid strength and pKa

Hybridization effect
Topic IV. Stereochemistry

• Isomers

Isomers: different compounds with the same molecular formula

Constitutional isomers

Stereoisomers

Diastereomers

Enantiomers
Topic IV. Stereochemistry

• **Isomers**

\[ \text{CH}_3\text{CH=CHCH}_3 \]
Topic IV. Stereochemistry

• **Chiral and Achiral**

Chiral: a molecule that is not superimposable on its mirror
Topic IV. Stereochemistry

• Chiral and Achiral
Topic IV. Stereochemistry

• Chiral and Achiral
Topic IV. Stereochemistry

• Stereogenic Center

```
Br

H  Cl
H  F

H  Cl
H  F

H  Cl
H  F
```
Topic V. Others

• Newnam Projection

[Images of eclipsed and staggered conformations of a molecule]
• Chair conformation:
Topic V. Others

• Chair conformation:
Topic V. Others

• Four key types of reactions:
  
  SN1

  SN2

  E1

  E2
Topic V. Others

• Oxidation state: