Chem 343  Summer 2002

Lecture 5

Topics

Overview of Functional Groups (cont.)
- recap on alkyl halides & alcohols
- ethers
- amines
- aldehydes and ketones
- carboxylic acids
- esters
- amides
- nitriles

Polar Covalent Bonds and Dipole Moments
Intramolecular Forces
- ion-ion
- dipole-dipole
- hydrogen bonding
- Vander Waals Forces (London Forces)
D. Alcohols \( R - OH \)

Can be thought of as hydroxy substituted alkanes or alkyl substituted water.

Examples:
- Methanol \( \text{CH}_3\text{OH} \)
- Ethanol \( \text{CH}_3\text{CH}_2\text{OH} \) \( 1^\circ \) alcohol
- Isopropanol \( \text{CH}_3\text{CH}-\text{CH}_3 \) \( 2^\circ \) alcohol
- \( \epsilon \)-Butanol
  \[ \text{CH}_3 \]
  \[ \text{H}_3\text{C}-\text{C}-\text{OH} \]
  \[ \text{CH}_3 \]
  \( 3^\circ \) alcohol

E. Ethers \( R - O - R \)

Examples:
- Dimethyl ether \( \text{CH}_3\text{OCH}_3 \)
- Diethyl ether \( \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 \)

May be cyclic with 0 part of ring

- Ethylene oxide
- Tetrahydrofuran (THF)
Amines - $RNH_2$, $R_2NH$, $R_3N$

can be thought of as alkyl-substituted ammonia.

Also classified as primary, secondary, tertiary, but these terms are defined differently for amines. Primary, secondary, tertiary refer to the number of carbon groups attached to the amine nitrogen.

Examples:

$H_2NCH_3$ methylamine 1° amine

$CH_3-CH_2$N$\cdot$H$_2$ isopropylamine 1° amine

$NH_2$

$(CH_3CH_2)_2$NH diethylamine 2° amine

$CH_3$

$CH_2-CH-NH_2$ (R)amphetamine 1° amine

$(CH_3CH_2)_3$N triethylamine 3° amine
G. Aldehydes and Ketones

1. contain carbonyl group

aldehyde: \( R - C = O - H \)
ketone: \( R - C - R \)

Examples:

- \( H - C - H \) formaldehyde
- \( CH_3 C - H \) acetaldehyde
- \( CH_3 - C - CH_3 \) acetone

H. Carboxylic Acids: \( R - C - O - H \)

- \( H - C - O - H \) formic acid
- \( CH_3 - C - O - H \) acetic acid
- \( \text{benzoic acid} \)
I. Esters $R - C - O - R$

Formed from carboxylic acid plus alcohol by eliminating water:

\[ CH_3-C-OH + HO-CH_2-CH_3 \rightarrow CH_3-C-O-CH_2CH_3 \]

- acetic acid
- ethanol
- ethyl acetate.

Other examples:

\[ \text{cyclic structure} \quad \text{methyl benzoate} \]

\[ CH_3CH_2C-O-C\text{I} \quad \text{isopropyl propionate} \]

J. Amides

Formed from carboxylic acid plus amine by eliminating water:

\[ CH_3-C-OH + H+\text{N}-H \rightarrow CH_3-C-NH_2 \]

- acetic acid + ammonia
- acetamide
K. Nitriles  \( R-C\equiv N \)
contain sp carbon with triple bond to nitrogen.

Examples:
\[ CH_3-C\equiv N \]  ethynenitrile (acetoneitrile)
\[ H_2C\equiv CH-C\equiv N \]  propenenitrile (acrylonitrile)

L. Summarize via Table 2.3.

III.

A. Polar Covalent Bonds

1. Electronegativity - ability of an atom to draw electrons toward itself in a covalent bond.

2. Covalent bonds between two different elements will be at least somewhat polarized due to uneven sharing of e-'s.

<table>
<thead>
<tr>
<th>( \Delta EN )</th>
<th>bond type</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 - 0.5</td>
<td>covalent</td>
</tr>
<tr>
<td>0.5 - 2.0</td>
<td>polar covalent</td>
</tr>
<tr>
<td>&gt; 2.0</td>
<td>ionic</td>
</tr>
</tbody>
</table>
B. Dipole Moment

1. The presence of polar covalent bonds in a molecule may or may not lead to an overall uneven charge distribution.

2. When there is an overall uneven distribution of charge, the molecule is said to have a dipole moment defined by

   \[ \mu = e \times d \]

   where \( e \) = charge in esu
   
   \( d \) = distance of charge separation in cm

3. The direction and relative magnitude of dipole moments can be predicted from EN values and molecular geometry.

   examples: \( \text{H}_2\text{O} \)

   \[ \begin{array}{c}
   \mu \\
   \text{O} \\
   \text{H} \end{array} \]

   example: \( \text{C}_2\text{O}_2 \)

   \[ \begin{array}{c}
   \text{O} = \text{C} = \text{O} \\
   \mu = 0 \end{array} \]
example: $\text{Cl}_2 + \text{Cl}_2$

\[\begin{array}{c}
\text{Cl} \\
\downarrow \\
\text{C} \\
\downarrow \\
\text{H} \\
\uparrow \\
\text{H} \\
\end{array}\]

example:

\[\begin{array}{c}
\text{F} \\
\downarrow \\
\text{B} \\
\text{F} \\
\end{array}\]

$\mu = 0$

example. cis - $\text{CH}_2\text{F}_2 = \text{CH}_2\text{F}$

\[\begin{array}{c}
\text{F} \\
\downarrow \\
\text{C} \\
\downarrow \\
\text{H} \\
\end{array}\]

\[\begin{array}{c}
\text{F} \\
\downarrow \\
\text{C} \\
\downarrow \\
\text{H} \\
\end{array}\]

$\mu = 0$

trans - $\text{CH}_2\text{F}_2 = \text{CH}_2\text{F}$

\[\begin{array}{c}
\text{H} \\
\downarrow \\
\text{C} = \text{C} \\
\text{F} \\
\downarrow \\
\text{H} \\
\end{array}\]

$\mu = 0$
IV. Intermolecular Forces

A. Ion - Ion

1. Very strong attractive forces occur between positively and negatively charged ions.

2. Ionic bonding, as previously mentioned, results in high melting crystalline compounds.

Example:

\[
\begin{align*}
\text{CH}_3\text{C}^+\text{OH} & \quad \xrightarrow{\text{NaOH}} \quad \text{CH}_3\text{C}^-\text{O}^\circ \text{Na}^+ \\
\text{m.p.} & \quad 16.6 \degree \text{C} \\
\text{b.p.} & \quad 118 \degree \text{C}
\end{align*}
\]

m.p. 324 \degree \text{C}

b.p. (above close temp.)

B. Dipole - Dipole

1. Although much weaker than ion-ion forces, dipole-dipole forces strongly affect the physical properties of organic compounds.

2. Molecules with larger dipole will generally have higher boiling points.
Examples:

\[
\begin{align*}
\ce{H3C-O-CH3} & \quad \text{b.p. } -25^\circ C \\
\ce{CH3-CH2-CH2-CH3} & \quad \text{b.p. } 35^\circ C
\end{align*}
\]

\[
\begin{align*}
\ce{CH3-C(CH3)3} & \quad \text{b.p. } 56^\circ C \\
\ce{CH3-C(CH3)3} & \quad \text{b.p. } 102^\circ C
\end{align*}
\]

C. Hydrogen Bonding - Special Case of Dipole-dipole attraction.

When a hydrogen is bonded to a strongly electronegative atom, which also has non-bonding electron pairs on a strongly electronegative atom form particularly strong dipole-dipole interactions known as hydrogen bonds.

Examples:

\[
\begin{align*}
\ce{H-N::H} & \\
\ce{CH3-O-H\ldots-O-H}\quad \text{b.p. } 102^\circ C
\end{align*}
\]