Read Chapter 12

1H NMR pgs. 348-359

We'll start this on Friday

Problem sets are due in class on Friday.

Formulas

\[ \text{C}_4\text{H}_{10} \rightarrow \text{H}_3\text{C}(\text{CH}_3)_2\text{CH}_3 \rightarrow \text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_3 \rightarrow \]

"0 dimensions"

"very little info"

1D

2 dimensions

\[ \text{H}_3\text{C} \]

\[ \text{CH}_3 \]

3 dimensions

Out towards you

Time - The 4th Dimension

- Rotation - around bonds

- Vibration - along bonds

\[ \text{H}_3\text{C}-\text{CH}_2 \]

\[ \text{CH}_3 \]

What information can you get from a formula?

\[ \text{C}_5\text{H}_8 \text{O}_2 \]

(# of rings + \( \pi \) bonds) = "unsaturations"

\[ \text{C} \equiv \text{C}^\equiv \text{H} \]

\[ \text{C} \equiv \text{C} \]

\[ \text{H} \]

\( \pi \) bonds from

\( \sigma \) bond

\( \rho \) orbitals

write on this side only - do not double side for genchem office
Every time you make a ring or a double bond, it "costs" 2 hydrogens.

\[ \text{by figuring out how many Hs are missing we can find out how many rings or double bonds the molecule has.} \]

"Full" = C\text{N} \text{H}_{2n+2} \quad \text{for } \text{C}_5 \text{H}_8 \text{O}_2 \text{ we have}

\[ 2(5) + 2 = 12 \quad 12 - 8 = 4 \text{ H missing} \]

Nitrogens need one more H; Oxygens don't change; Chlorine or Br count as Hs.

Someone drew: (someone brave)

\[ \text{also works} \]

Sod many others.
Best Lewis Structure

1) $8\text{e}^-$ at each C, N, O
2) Negative charge on most electronegative element

\[ \begin{array}{c}
\text{H} & : & \text{C} & : & \text{H} \\
\text{H} & : & \text{N} & : & \text{H} \\
\text{H} & : & \text{O} & : & \text{H}
\end{array} \]

Best curved arrows

\[ \Rightarrow \begin{array}{c}
\text{H} & \Rightarrow & \text{C} & \Rightarrow & \text{H} \\
\text{H} & \Rightarrow & \text{N} & \Rightarrow & \text{H} \\
\text{H} & \Rightarrow & \text{O} & \Rightarrow & \text{H}
\end{array} \]

Formal Charge

\[ \begin{array}{c}
\text{C} & : & \text{H} & : & \text{H} \\
\text{H} & : & \text{N} & : & \text{H} \\
\text{H} & : & \text{O} & : & \text{H}
\end{array} \]

\[ \begin{array}{c}
\text{C} & : & \text{H} & : & \text{H} \\
\text{H} & : & \text{N} & : & \text{H} \\
\text{H} & : & \text{O} & : & \text{H}
\end{array} \]

So... Formaldehyde Looks mostly like \( \begin{array}{c}
\text{H} \\
\text{H}
\end{array} \) but a little like \( \begin{array}{c}
\text{H} \\
\text{H}
\end{array} \)

More resonance structures -> more stable molecule
Energies of resonance structures.

\[ \text{Real Energy} \]

\[ H - C : O \quad \leftrightarrow \quad H - O - C \quad \leftrightarrow \quad H - C : B \]

A, B, and C are the same and much better than B. The real structure is directly between and lower in energy than either.

<table>
<thead>
<tr>
<th># of atoms on C</th>
<th>Orbitals</th>
<th>Dimensions</th>
<th>Shape</th>
<th>Angles</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>2s 2p(3p) 2p(3p)</td>
<td>3</td>
<td>Tetrahedral</td>
<td>109°</td>
</tr>
<tr>
<td>3</td>
<td>2s(2p) 2p(3p)</td>
<td>2</td>
<td>Flat</td>
<td>120°</td>
</tr>
<tr>
<td>2</td>
<td>2s, 2p</td>
<td>1</td>
<td>Linear</td>
<td>180°</td>
</tr>
</tbody>
</table>
Next time: NMR spectroscopy and IR spectroscopy.

- NMR spectroscopy: looks at hydrogen nuclei and their magnetic properties.
- IR spectroscopy: looks at stretching of bond vibrations.