Introduction to Spectroscopy

Electromagnetic Radiation:

\( \lambda \)

\( \nu \)

E

h

c

Fundamental equations:

You must know the relative ordering of the various regions of the electromagnetic spectrum:

___________________________________________________________________________

\[ \lambda \quad E, \nu \]

___________________________________________________________________________

Important: What is the wavelength range of visible light?

The way the electromagnetic radiation interacts with molecules depends upon its energy:

___________________________________________________________________________

<table>
<thead>
<tr>
<th>UV/VIS</th>
<th>IR</th>
<th>NMR</th>
</tr>
</thead>
</table>

___________________________________________________________________________
Infrared Spectroscopy

1. Units used for IR Spectroscopy:

   Wavelength:

   Frequency:

2. When IR light is absorbed by a molecule, the molecule changes its ___________________.

   There are two types of molecular vibrations: _______________ and _______________.

   Examples:

   \[ \text{H-Cl} \rightleftharpoons h\nu \]

   What happens to the center of mass of H-Cl?

   \[ \text{O=\text{C}=\text{O}} \]

   Therefore, CO₂ has 3 vibrational modes.

   Ethanol (CH₃CH₂OH) has 21 possible vibrations (theoretically), but most are for C-H vibrations.

3. Importance of Polarity

   Not all molecular vibrations absorb IR radiation.

   A **non-polar bond** does not absorb IR radiation. Examples:

   A **polar bond** does absorb IR radiation. Example:
Only unsymmetrically substituted bonds have dipole moments and are infrared active.

Examples:  **IR Active:**

**Not IR Active:**

4. The frequency of a stretching vibration is related to:

1)

2) In general, the lighter the atoms, the ______________ the frequency.

   In general, the stronger the bond, the ______________ the frequency.

**Interpreting IR Spectra**

1. Know the general regions in the IR spectrum.

2. Know the appearance of an IR spectrum:
3. Look for distinctive absorptions (“landmarks”). (Memorize these numbers.)

1)

2)

3)

4)

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**NMR Spectroscopy**

An NMR spectrum provides four kinds of information:

1.

2.

3.

4.
1. Principle: Protons in different environments are magnetically nonequivalent and absorb energy at different frequencies. Therefore, the number of signals indicates how many kinds of protons are in a molecule.

Examples: Determine the number of nonequivalent protons in the following compounds.

\text{CH}_3\text{-CH}_2\text{-Cl}

\text{Br-CH}_2\text{-CH}_2\text{-Br}

\text{F-CH}_2\text{-CH}_2\text{-Br}

\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-CHO}

2. The positions of the signals. The chemical shift value indicates the electronic environment of the protons.

<table>
<thead>
<tr>
<th>(\delta)</th>
<th>type of proton</th>
</tr>
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3. The intensity of the signal indicates how many protons of each kind.

Indicate the number of signals and the relative intensity of each signal in the following molecules:

$$\text{CHCl}_2\text{-CH}_3$$

$$\text{Br-CH}_2\text{-CH-(CH}_3)_2$$

4. The splitting of the signal tells us about the adjacent protons.

What would be the splitting of each proton in the molecules below?

$$\text{CH}_3\text{-CH}_2\text{-Cl}$$

$$\text{F-CH}_2\text{-CH}_2\text{-Br}$$

$$\begin{array}{c}
\text{O} \\
\text{H}_3\text{C}--\text{C}--\text{CH}--\text{CH}_3
\end{array}$$

$$\text{Cl-CH}_2\text{-CH}_2\text{-Cl}$$
The general appearance of a proton NMR spectrum.

**Identify**: TMS, upfield, downfield, shielded, deshielded in the spectrum below:

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5                      4                      3                      2                      1                      0
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**Examples**: Predict the NMR spectra of the compounds below.

1. \( \text{CH}_2 - \text{CH}_2 \)
2. \( \text{CH}_3\text{-CHBr}_2 \)

3. \( \text{CH}_3\text{-CH}_2\text{-Br} \)
4. \( \text{CH}_3-\text{CH-CH}_3 \)

5. \( \begin{array}{c}
\text{H}_3\text{C} \\
\text{CH-O-C--CH}_2\text{CH}_3
\end{array} \)