Number of vibrations equal 3N-6

3 coordinates for each atom minus
three translations and three rotations

Exam 2 is next Wednesday Evening, October 25
The TAs will have review sessions Monday from 7:00-9:00pm
Two rooms - Old Chem 116, and Harriman 137

Reading assignments for Spectroscopy
Chapter 12 - Infrared: pages 474-489
Chapter 13 - NMR pages: 493-521 + 527-532
Chapter 14 - Mass Spec - pages: 543-551

To interact with light the vibration must change the
dipole of the molecule.

http://www.cm.ceu.edu/~reusch/VirtualText/Specopy/InfraRed/infrared.html#r

Introduction to Spectroscopy

Symmetric stretching
Asymmetric stretching
Stretching vibrations

Scissoring
Wagging
Twisting
Bending vibrations

Table 13.1 Wavelengths, Frequencies, and Energies of Some Regions of the Electromagnetic Spectrum

nuclear transformations
core electron excitations
molecular vibrations
molecular rotations

nuclear spin flips

light

modes
Nuclear Magnetic Resonance.

All of these hydrogen atoms have a magnetic moment.

Nuclear Magnetic Resonance.

These magnetic moments have no orientation.

Table 1.3.1 Spin Quantum Numbers and Allowed Nuclear Spin States for Selected Isotopes of Elements Common to Organic Compounds

Any nucleus that has an odd atomic number or an odd mass number or both has a nuclear magnetic moment (nuclear spin).

NMR
Nuclear Magnetic Resonance.
In a magnetic field the hydrogen nuclei orient parallel and antiparallel to the magnetic field.

\[
\begin{align*}
N & \quad T_{\text{axol}} \\
& \quad C_{47}H_{51}NO_{14}
\end{align*}
\]

Nuclear Magnetic Resonance.
more of the hydrogen nuclei are oriented parallel than antiparallel to the magnetic field.

\[
\begin{align*}
\text{the molecules absorb light of an energy equal to the energy difference between the two spin states.} \\
\Delta \varepsilon & = 300 \text{ MHz} = 300,000,000 \\
\Delta \varepsilon & = 0.12 \text{ J/mol} \\
\Delta \varepsilon (H-H \text{ bond}) & = 436,000 \text{ J/mol}
\end{align*}
\]

Nuclear Magnetic Resonance.
The different hydrogen nuclei in a molecule experience different magnetic fields due to shielding.

\[
\begin{align*}
\text{Down field, weaker magnetic field} & \quad \text{Up field, stronger magnetic field}
\end{align*}
\]
Because the electrons can alter the magnetic field in different regions of a molecule.

Nuclear Magnetic Resonance.

the different hydrogen nuclei in a molecule experience different magnetic fields due to shielding.

The molecules absorb light of an energy equal to the energy difference between the two spin states.

\[
\Delta E = 300 \text{ MHz} = 300,000,000 \text{ Hz}
\]

\[
\Delta E = 300,000,300 \text{ Hz}
\]

\[
\Delta E - \Delta E = 300 \text{ Hz}
\]

Because the electrons can alter the magnetic field in different regions of a molecule.

an NMR spectrum at 300 MHz

\[
\frac{300 \text{ Hz}}{300,000,000} = 1.0 \text{ ppm}
\]

\[
\frac{300,000,300 \text{ Hz}}{300 \text{ Hz}}
\]

\[
\Delta E = 300 \text{ MHz} = 300,000,000 \text{ Hz}
\]

\[
\Delta E = 300,000,300 \text{ Hz}
\]

\[
\Delta E - \Delta E = 300 \text{ Hz}
\]

The magnetic field experienced by a given proton depends upon the relationship to the other magnetic fields in a molecule.

Why do different hydrogen nuclei in an organic molecule experience a different magnetic field?
### Chemical Shift

<table>
<thead>
<tr>
<th>Type of Hydrogen</th>
<th>Chemical Shift (ppm)</th>
<th>Type of Hydrogen</th>
<th>Chemical Shift (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rx</td>
<td>0.0–0.8</td>
<td>O</td>
<td>3.7–3.9</td>
</tr>
<tr>
<td>R$_1$H$_2$</td>
<td>1.2–1.4</td>
<td>R$_2$OCH$_3$</td>
<td>3.7–4.3</td>
</tr>
<tr>
<td>R$_2$CH</td>
<td>1.6–2.7</td>
<td>R$_2$OCH$_3$</td>
<td>3.7–4.3</td>
</tr>
<tr>
<td>R$_2$C(O)CH$_3$</td>
<td>2.8–3.0</td>
<td>R$_2$OCH$_3$</td>
<td>3.7–3.9</td>
</tr>
<tr>
<td>A-C$_3$H$_7$</td>
<td>2.3–2.8</td>
<td>R$_2$OCH$_3$</td>
<td>3.7–4.3</td>
</tr>
<tr>
<td>R$_3$O</td>
<td>3.5–4.0</td>
<td>R$_3$O$_2$</td>
<td>4.4–5.5</td>
</tr>
<tr>
<td>R$_3$OCH</td>
<td>5.5–5.9</td>
<td>R$_3$O$_2$</td>
<td>4.4–5.5</td>
</tr>
<tr>
<td>R$_4$CH$_2$</td>
<td>5.6–5.9</td>
<td>R$_4$O$_2$</td>
<td>4.4–5.5</td>
</tr>
<tr>
<td>R$_5$</td>
<td>9.5–10.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>R$_5$OCH$_3$</td>
<td>2.2–2.6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Taxol**

C$_{47}$H$_{53}$NO$_{14}$