Problem R-03C (C₇H₁₀O)
300 MHz ¹H NMR Spectrum in CDCl₃
Source: Olafs Daugulis/T. Walker/Vedejs 10/26 g

IR Spectrum
Problem R-03C ($\text{C}_7\text{H}_{10}\text{O}$)

75.46 MHz $^{13}$C NMR Spectrum in CDCl$_3$

The top spectrum is DEPT 135, with CH$_2$ negative, CH, CH$_3$ positive.

Source: Olafs Daugulis/T. Walker/Vedejs 10/26
Problem R-03C (C₇H₁₀O). Determine the structure (or part structure) of R-03C from the ¹H NMR, ¹³C NMR and IR spectra provided.

(a) DBE_______

(b) What information can you obtain from the IR spectrum? Give frequency and assignment.

(c) Interpret the ¹³C NMR spectrum. The DEPT 135 spectrum shows all CH and CH₃ peaks as positive, and CH₂ peaks negative. Identify what kind of carbon each signal corresponds to, and write possible part structures.

<table>
<thead>
<tr>
<th>Type of C (e.g. sp³ CH₃) and/or part structures (e.g. N-CH₂)</th>
<th>δ 21.0</th>
<th>δ 27.8</th>
<th>δ 122.0</th>
<th>δ 127.0</th>
<th>δ 138.2</th>
<th>δ 157.0</th>
<th>δ 190.3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(d) What are the three peaks at δ 77? _______________________________
(e) Assign and analyze the signals between $\delta$ 1.9 and 2.2 in the 300 MHz $^1$H NMR spectrum. Report multiplicity, coupling constants and part structure you could obtain from each signal.

(f) Analyze the multiplets between $\delta$ 5.7 and 6.45. Report multiplicity, coupling constants and part structure you could obtain from each signal (in the standard form: e.g., $\delta$ 3.9, tq, $J = 12$, 4 Hz, 1H). You may use first-order analysis.

(g) Draw the structure of R-03C. If more than one structure is possible, show them, and circle the one you think fits the data best and give your reasons for choosing it.
Problem R-03C (C_7H_{10}O). Determine the structure (or part structure) of R-03C from the \( ^1H \) NMR, \( ^{13}C \) NMR and IR spectra provided.

(a) DBE \( ^3 \)

(b) What information can you obtain from the IR spectrum? Give frequency and assignment.

(c) Interpret the \( ^{13}C \) NMR spectrum. The DEPT 135 spectrum shows all CH and CH\(_3\) peaks as positive, and CH\(_2\) peaks negative. Identify what kind of carbon each signal corresponds to, and write possible part structures.

<table>
<thead>
<tr>
<th>Type of C (e.g. sp(^3) CH(_2))</th>
<th>( \delta )</th>
<th>( ^{13}C ) NMR peaks</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH(_2)-C</td>
<td>( 21.0 )</td>
<td>( 21.0 )</td>
</tr>
<tr>
<td>CH(_3)-C</td>
<td>( 27.8 )</td>
<td>( 27.8 )</td>
</tr>
<tr>
<td>( C=CH )</td>
<td>( 122.0 )</td>
<td>( 122.0 )</td>
</tr>
<tr>
<td>( C=CH )</td>
<td>( 127.0 )</td>
<td>( 127.0 )</td>
</tr>
<tr>
<td>( C=CH )</td>
<td>( 138.2 )</td>
<td>( 138.2 )</td>
</tr>
<tr>
<td>( C=CH )</td>
<td>( 157.0 )</td>
<td>( 157.0 )</td>
</tr>
<tr>
<td>( C=CH )</td>
<td>( 190.3 )</td>
<td>( 190.3 )</td>
</tr>
</tbody>
</table>

These are the CDCl\(_3\) peaks (C split by D, \( I = 1 \))

(d) What are the three peaks at \( \delta \) 77? \( 3020 \text{ cm}^{-1} \) Vinyl CH stretch

No OH or \( C=O \)

1605 cm\(^{-1} \) C=C stretch

1680 cm\(^{-1} \) C=O stretch - conj ketone

3800 3600 3400 3200 3000 2800 2600 2400 2200 2000 1800 1600 1400 1200 1000 800 600 cm\(^{-1} \)
(e) Assign and analyze the signals between $\delta$ 1.9 and 2.2 in the 300 MHz $^1$H NMR spectrum. Report multiplicity, coupling constants and part structure you could obtain from each signal.

Two CH$_3$ groups, each split into a d, $J$ = 1.3 Hz

Chemical shifts suggests CH$_3$ on double bond or aryl ring

(f) Analyze the multiplets between $\delta$ 5.7 and 6.45. Report multiplicity, coupling constants and part structure you could obtain from each signal (in the standard form: e.g., $\delta$ 3.9, tq, $J$ = 12, 4 Hz, 1H). You may use first-order analysis.

$\delta$ 6.40 dd, $J$ = 17.5, 10.4 Hz. A part of ABX (trans and cis vivyl coupling)

$\delta$ 6.21 dd, $J$ = 17.5, 1.5 Hz. B part of ABX (trans and gem)

$\delta$ 5.74 dd, $J$ = 10.4, 1.5 Hz. X part of ABX (cis and gem)

$\delta$ 6.29, septet, $J$ = 2 Hz: vinyl proton split by 6 protons with small J - coupled to both CH$_3$ groups

(g) Draw the structure of R-03C. If more than one structure is possible, show them, and circle the one you think fits the data best and give your reasons for choosing it.

+ 10 other structures