Problem R-94C (C\textsubscript{12}H\textsubscript{14}O)
200 MHz $^1$H NMR spectrum in CDCl$_3$
Source: Carl Hoeger (Reich digitized hard copy)

![Chemical structure diagram](Image)

50 MHz $^{13}$C NMR spectrum in CDCl$_3$
**Problem R-94C.** \((C_{12}H_{14}O)\). Determine the structure (or part structure) of **R-94C** from the \(^1H\) NMR, \(^{13}C\) NMR and IR spectra provided.

(a) DBE \(\_\)  
(b) What information can you obtain from the IR spectrum? List the data, and any conclusions you drew from it.

(c) Analyze the \(^1H\) NMR signals. For each of the signals listed below report integration, multiplicity and coupling constants to the extent the signals are amenable to first order analysis, and the part structure each corresponds to.

\[
\begin{align*}
\delta 0.9 & \quad \delta 2.5 \\
\delta 1.1 & \quad \delta 7.5 \\
\delta 1.3 & \quad \delta 7.9 \\
\delta 1.5 & 
\end{align*}
\]

(c) Interpret the \(^{13}C\) NMR spectrum. Identify what kind of carbon each signal corresponds to, and write possible part structures.

<table>
<thead>
<tr>
<th>No</th>
<th>ppm</th>
<th>Type of C (e.g. sp(^3) CH(_2)) and/or part structures (e.g. N-CH(_2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>198.38 (s)</td>
<td>___________</td>
</tr>
<tr>
<td>2</td>
<td>139.08 (s)</td>
<td>___________</td>
</tr>
<tr>
<td>3</td>
<td>132.30 (d)</td>
<td>___________</td>
</tr>
<tr>
<td>4</td>
<td>128.40 (d)</td>
<td>___________</td>
</tr>
<tr>
<td>5</td>
<td>127.89 (d)</td>
<td>___________</td>
</tr>
</tbody>
</table>

(d) Determine the structure of R-94C. If more than one structure is possible, show them, and circle your best choice.
Problem R-94C (C_{12}H_{14}O)

200 MHz $^1$H NMR spectrum in CDCl$_3$

Source: Carl Hoeger (Reich digitized hard copy)

50 MHz $^{13}$C NMR spectrum in CDCl$_3$
Problem R-94C. \((C_{12}H_{14}O)\). Determine the structure (or part structure) of R-94C from the \(^1H\) NMR, \(^{13}C\) NMR and IR spectra provided.

(a) DBE 6

(b) What information can you obtain from the IR spectrum? List the data, and any conclusions you drew from it.

- 1680 cm\(^{-1}\) conjugated ketone C=O stretch
- 3050 cm\(^{-1}\) Vinyl/aryl C-H stretch
- Absence of peaks above 2300 cm\(^{-1}\) - no OH in molecule

(c) Analyze the \(^1H\) NMR signals. For each of the signals listed below report integration, multiplicity and coupling constants to the extent the signals are amenable to first order analysis, and the part structure each corresponds to.

\[
\begin{align*}
\delta & \quad 0.9 \quad \text{dd,} \ J = 7.7, 3.6 \text{ Hz,} \ 1\text{H} \\
\text{Coupled to} & \ \delta 1.5 \text{ and 2.5} \\
\delta & \quad 1.1 \quad \text{s,} \ 3\text{H} \ \text{C-CH}_3 \\
\delta & \quad 1.3 \quad \text{s,} \ 3\text{H} \ \text{C-CH}_3 \\
\delta & \quad 1.5 \quad \text{dd,} \ J = 5.5, 4.3 \text{ Hz,} \ 1\text{H} \\
\text{Coupled to} & \ \delta 0.9 \text{ and 2.5}
\end{align*}
\]

The multiplets at \(\delta 0.9, 1.5, 2.5\) are an isolated AMX pattern, coupled to nothing else

(c) Interpret the \(^{13}C\) NMR spectrum. Identify what kind of carbon each signal corresponds to, and write possible part structures.

<table>
<thead>
<tr>
<th>No</th>
<th>ppm</th>
<th>Type of C (e.g. sp(^3) CH(_2)) and/or part structures (e.g. N-CH(_2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>198.38 (s)</td>
<td>O (\text{Not aldehyde})</td>
</tr>
<tr>
<td>2</td>
<td>139.08 (s)</td>
<td>C (\text{s ipso aromatic})</td>
</tr>
<tr>
<td>3</td>
<td>132.30 (d)</td>
<td>C-H aromatic (para)</td>
</tr>
<tr>
<td>4</td>
<td>128.40 (d)</td>
<td>C-H aromatic (\text{ortho and meta double intensity})</td>
</tr>
<tr>
<td>5</td>
<td>127.89 (d)</td>
<td>C-H aromatic (\text{ortho and meta double intensity})</td>
</tr>
<tr>
<td>6</td>
<td>32.82 (d)</td>
<td>sp(^3) tertiary</td>
</tr>
<tr>
<td>7</td>
<td>26.98 (q)</td>
<td>(\text{C-CH}_3)</td>
</tr>
<tr>
<td>8</td>
<td>26.81 (s)</td>
<td>sp(^3) quaternary unusually upfield</td>
</tr>
<tr>
<td>9</td>
<td>21.96 (t)</td>
<td>(\text{sp}(^3) C-CH(_2)-C)</td>
</tr>
<tr>
<td>10</td>
<td>18.43 (q)</td>
<td>(\text{C-CH}_3)</td>
</tr>
</tbody>
</table>

The 4 signals 127-139 form a monosubstituted benzene

(d) Determine the structure of R-94C. If more than one structure is possible, show them, and circle your best choice.

There is the benzene ring and two more unsaturations - one is the ketone, the other must be a ring.

Other proposed structures

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