Problem R-07F (C₈H₁₄O₄)
300 MHz ¹H NMR spectrum
Source: Aldrich Spectra Collection/Reich g

Problem R-07F (C₈H₁₄O₄)
75 MHz ¹³C NMR spectrum
Source: Aldrich Spectra Collection
**Problem R-07F** \((C_8H_{14}O_4)\). Determine the structure of the compound from the \(^1H\) and \(^{13}C\) NMR spectra given.

(a) DBE____

(b) The IR spectrum shows a strong signal at 1735 cm\(^{-1}\). What does this tell you?

(c) Interpret the \(^{13}C\) NMR spectrum. Use the Normal, DEPT-135 and DEPT 90 spectra to help in the analysis. Identify what kind of carbon each signal corresponds to and write possible part structures (you may wish to examine all the data before completing this section).

Type of C (e.g. sp\(^3\) CH\(_2\)) and/or part structures (e.g. N-CH\(_2\))

<table>
<thead>
<tr>
<th>ppm</th>
<th>18.5</th>
<th>25.6</th>
<th>27.1</th>
<th>52.1</th>
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</thead>
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<tr>
<th>ppm</th>
<th>75.0</th>
<th>80.3</th>
<th>110.4</th>
<th>170.8</th>
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(d) Interpret the \(^1H\) signals between \(\delta 4.0\) and 4.4. Give part structures, shifts, and any couplings

(d) Draw the structure of **R-07F**. 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-07F (C₈H₁₄O₄). Determine the structure of the compound from the ¹H and ¹³C NMR spectra given.

(a) DBE

(b) The IR spectrum shows a strong signal at 1735 cm⁻¹. What does this tell you?

There is a carbonyl in the molecule, probably an ester or lactone

(c) Interpret the ¹³C NMR spectrum. Use the Normal, DEPT-135 and DEPT 90 spectra to help in the analysis. Identify what kind of carbon each signal corresponds to and write possible part structures (you may wish to examine all the data before completing this section).

<table>
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<th>(e.g. sp³ CH₂) and/or part structures (e.g. N-CH₂)</th>
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</thead>
<tbody>
<tr>
<td>18.5</td>
<td>sp³ H-C-O</td>
</tr>
<tr>
<td>25.6</td>
<td>sp³ H-C-O</td>
</tr>
<tr>
<td>27.1</td>
<td>sp³ C(OR)₂, possible -C≡C-</td>
</tr>
<tr>
<td>52.1</td>
<td>sp² O=C-OR, ester carbonyl</td>
</tr>
</tbody>
</table>

(d) Interpret the ¹H signals between δ 4.0 and 4.4. Give part structures, shifts, and any couplings.

The chemical shift requires α-oxygen substituents or possibly vinyl protons), the couplings shows an isolated CH₃-CH-CH spin system

(d) Draw the structure of R-07F. 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.

These two also fit the NMR data
Problem R-07F (C₈H₁₄O₄)
300 MHz ¹H NMR spectrum
Source: Aldrich Spectra Collection

Problem R-07F (C₈H₁₄O₄)
75 MHz ¹³C NMR spectrum
Source: Aldrich Spectra Collection

DEPT 90

DEPT 135

Normal