Structure Determination using NMR and IR Spectral Data

Click on a number to view the spectral data for each compound.

Data for each unknown includes: $^1$H NMR (splitting patterns included)
$^{13}$C NMR
IR spectrum (KBr pellet or film)

Solvent peaks due to CDCl$_3$ are present at 7.2 ppm in the proton spectra and 77.0 ppm in the carbon spectra.

In the $^1$H NMR spectra, the phrase "exchanges" means that shaking the NMR solution with D$_2$O resulted in loss of the signal due to hydrogen/deuterium exchange.

Click here to learn about interpretation of spectral data.

<table>
<thead>
<tr>
<th></th>
<th>#1 C$_4$H$_6$O</th>
<th>#6 C$<em>8$H$</em>{19}$N</th>
<th>#11 C$<em>6$H$</em>{12}$O$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>#2</td>
<td>C$_3$H$_5$O$_2$Br</td>
<td>#7 C$_3$H$_7$OCl</td>
<td>#12 C$_3$H$_7$OCl</td>
</tr>
<tr>
<td>#3</td>
<td>C$<em>9$H$</em>{12}$</td>
<td>#8 C$_6$H$_8$O$_2$</td>
<td>#13 C$<em>8$H$</em>{11}$O$_2$Br</td>
</tr>
<tr>
<td>#4</td>
<td>C$<em>6$H$</em>{10}$</td>
<td>#9 C$_6$H$_4$Cl$_2$</td>
<td>#14 C$<em>{10}$H$</em>{12}$O$_2$</td>
</tr>
<tr>
<td>#5</td>
<td>C$_8$H$_8$O$_2$</td>
<td>#10 C$<em>{18}$H$</em>{35}$N</td>
<td>#15 C$<em>9$H$</em>{13}$NO</td>
</tr>
</tbody>
</table>
Interpretation of Data

Use the **molecular formula** to determine the degrees of unsaturation or double bond equivalents (rings or multiple bonds).

Most of the $^1$H spectra contain first-order splitting patterns; in cases where some peaks do not follow the $N+1$ rule, by process of elimination of other peaks, you can solve the problem. Look for the obvious first-order splitting patterns:

- ethyl pattern (triplet and quartet)
- isopropyl pattern (double and multiplet, which may resolve into a discernable heptet)
- methoxy groups on esters (singlet downfield from alkane region, approx. 3.5 ppm)
- methyl group adjacent to a carbonyl (approximately 2.0 ppm)
- aromatic signals along with at least 4 degrees of unsaturation indicates a benzene ring.

Examine the IR spectrum to determine the **functional groups** present in the unknown:

- For example, if the formula contains oxygen, you should be able to distinguish between an ether versus an alcohol (O-H stretch).
- If a carbonyl stretch is present, look for O-H stretch (acid) or N-H stretch (amide).
- Look for triple bonds at approximately 2200 cm$^{-1}$.
- Look for sp$^2$ carbon-hydrogen frequencies above 3000 cm$^{-1}$ (alkenes, aromatic rings).

Remember, the number of peaks in the $^{13}$C spectrum indicates the number of different kinds of carbon atoms, the magnetically different carbon atoms. Some of the $^{13}$C spectra contain carbon-hydrogen splitting information labeled as a **multiplet**.

For example, a peak listed as 38.6, t means the peak is at 38.6 ppm and exists as a triplet.

- A quartet indicates there are three hydrogens attached to that carbon atom (CH$_3$ group).
- A triplet indicates there are 2 hydrogens attached to that carbon atom (CH$_2$ group).
- A doublet indicates there is one hydrogen attached to that carbon atom (CH group).
- A singlet indicates a quaternary carbon group.
$^1$H NMR spectrum  $^{13}$C NMR spectrum  IR spectrum

#1  C$_4$H$_6$O

*peak splitting below*

3.72  t  2H
3.48  bs  1H (exchanges)
2.45  t  2H
2.08  s  1H

back to problems
$^1\text{H NMR spectrum}$  $^{13}\text{C NMR spectrum}$  IR spectrum

#1  $\text{C}_4\text{H}_6\text{O}$
$^1$H NMR spectrum  $^{13}$C NMR spectrum  IR spectrum

#1  $C_4H_6O$

back to problems
1H NMR spectrum  13C NMR spectrum  IR spectrum
#2  C₃H₆O₂Br  
<back to problems>

peak splitting below

1H very broad (exchanges)
#2  C$_3$H$_5$O$_2$Br

$^{1}H$ NMR spectrum  $^{13}C$ NMR spectrum  IR spectrum

178.5, s  38.5, t  24.3, t
#2 $\text{C}_3\text{H}_5\text{O}_2\text{Br}$
$^1$H NMR spectrum  $^{13}$C NMR spectrum  IR spectrum

$^3$ C$_9$H$_{12}$

peak splitting below

back to problems
1H NMR spectrum  13C NMR spectrum  IR spectrum

#3  C₉H₁₂

back to problems
#4  C₆H₁₀

all singlets!

back to problems
1H NMR spectrum  
13C NMR spectrum  
IR spectrum

#4 C₆H₁₀

back to problems
#4  C₆H₁₀

IR spectrum

Transmittance

Wavenumber (cm⁻¹)

3064  2985  2790  1692  1372

3500  3000  2500  2000  1500  1000
#5  C₈H₆O₂

all singlets!
#5  C₈H₆O₂

back to problems
#5  
C₈H₆O₂

IR spectrum
$^{1}H$ NMR spectrum  $^{13}C$ NMR spectrum  IR spectrum

$C_{8}H_{19}N$

back to problems

peak splitting below
#6 \( \text{C}_8\text{H}_{19}\text{N} \)

\begin{align*}
49.8, t & \\
32.3, t & \\
20.4, t & \\
13.9, q & \\
\end{align*}
$^1$H NMR spectrum  $^{13}$C NMR spectrum  IR spectrum

#6  C$_8$H$_{19}$N

back to problems
#7  C$_3$H$_7$OCl

peak splitting below
1H NMR spectrum  13C NMR spectrum  IR spectrum

#7  C$_3$H$_7$OCl

back to problems
#7 C$_3$H$_7$OCl
$^1$H NMR spectrum  $^{13}$C NMR spectrum  IR spectrum

#8  C$_6$H$_6$O$_2$

*peak splitting below*
1H NMR spectrum  

13C NMR spectrum  

IR spectrum  

#8 $\text{C}_6\text{H}_6\text{O}_2$  

back to problems
#8  C₆H₆O₂

IR spectrum

Transmittance

Wavenumber (cm⁻¹)

335

1518

1364

1188

743
#9  C₆H₄Cl₂

peak splitting below
1H NMR spectrum  
13C NMR spectrum  
IR spectrum

#9  C₆H₄Cl₂  

back to problems
#9  C₆H₄Cl₂

IR spectrum

Transmittance

Wavenumber (cm⁻¹)

3500 3000 2500 2000 1500 1000

907 1458 1127 746
#10  \( C_{16}H_{35}N \)

**peak splitting below**
#10  \( \text{C}_{16}\text{H}_{35}\text{N} \)

back to problems
#10  C_{16}H_{35}N

IR spectrum

Transmittance

Wavenumber (cm$^{-1}$)

- 3727
- 2929
- 2854
#11  C\(_5\)H\(_{12}\)O\(_2\)  

*all singlets!*
#11  $C_5H_{12}O_2$
#11 $\text{C}_5\text{H}_{12}\text{O}_2$

IR spectrum
\[ \text{\(^1H\) NMR spectrum} \quad \text{\(^{13}C\) NMR spectrum} \quad \text{IR spectrum} \]

\#12 C\(_3\)H\(_7\)OCl

\text{peak splitting below}

1H (exchange)
\( \text{\( ^{1}H \) NMR spectrum} \)  \( \text{\( ^{13}C \) NMR spectrum} \)  \( \text{IR spectrum} \)

\#12  \( \text{C}_3\text{H}_7\text{OCl} \)

back to problems
#12  \( \text{C}_3\text{H}_7\text{OCl} \)

**Back to problems**
#13  C$_6$H$_{11}$O$_2$Br

peak splitting below
#13  C₆H₁₁O₂Br


1H NMR spectrum  
13C NMR spectrum  
IR spectrum

#13  C₆H₁₁O₂Br

back to problems
$^{1}H$ NMR spectrum

$^{13}C$ NMR spectrum

IR spectrum

#14 $C_{10}H_{12}O_{2}$

back to problems

peak splitting below
\[
\text{\textsuperscript{1}H NMR spectrum} \quad \text{\textsuperscript{13}C NMR spectrum} \quad \text{IR spectrum}
\]

\[\text{#14 } \text{C}_{10}\text{H}_{12}\text{O}_2\]

\[\text{back to problems}\]
#14  $C_{10}H_{12}O_2$

back to problems
#15  C$_9$H$_{13}$NO

Back to problems

Peak splitting below
#15  C$_9$H$_{13}$NO

1H NMR spectrum

13C NMR spectrum

IR spectrum

back to problems
#15  C\textsubscript{9}H\textsubscript{13}NO