

CHEM1002 Worksheet 5: Spectroscopy Workshop (2)

This worksheet forms part of the 'Spectroscopy Problem Solving Assignment' which represents 10% of the assessment of this unit. You should use the support material on eLearning alongside this worksheet and your lecture notes. The assignment is assessed through online quizzes and must be completed by the end of week 7.

Model 1: Mass Spectrometry

Mass spectrometry allows us to determine the molecular weight of a compound. However, it is a highly destructive technique, and molecules will often break up into smaller fragments. These fragments can further help in the identification of the compound. For example, a CH_2CH_3 group has a mass of 29, so a peak at 29 might indicate the presence of a CH_2CH_3 group.

Critical thinking questions

1. A compound containing carbon, hydrogen and nitrogen displays a molecular ion peak in its mass spectrum at m/z 41 and a fragment ion at m/z 15. Give the structure of a compound which is consistent with these data

Model 2: Combined Use of Mass Spectrometry and IR, UV-Visible and NMR Spectroscopy to Identify Unknown Compounds.

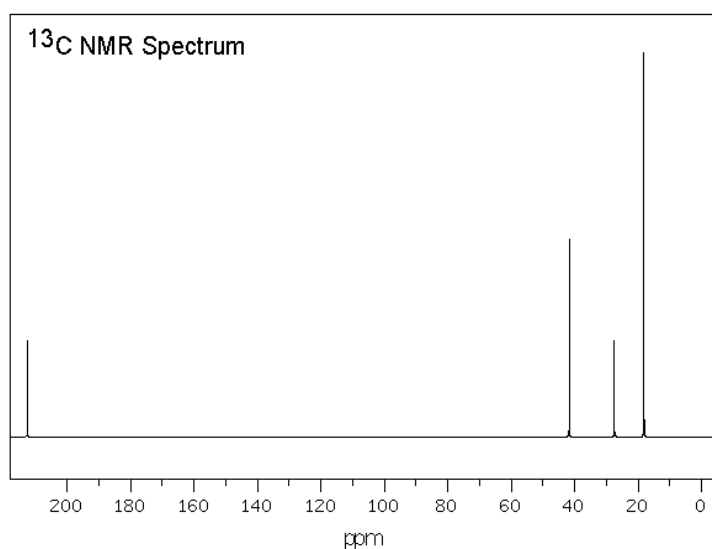
Commonly, all of these techniques are used to identify an unknown or newly synthesized compound as unambiguously as possible. The compound must be consistent with the results of *each* technique:

- mass spectrometry – helps to identify the molecular mass and, through the fragment pattern, can also be used to identify group that are present (such as $-\text{CH}_3$ or $-\text{C}_6\text{H}_5$).
- UV – Visible spectroscopy – identifies the presence / absence of conjugation such as aromatic rings
- IR spectroscopy – identifies the presence of common bonds, especially $\text{C}=\text{O}$ and $\text{O}-\text{H}$
- NMR – identifies types of atoms present (chemical shifts) and the presence of symmetry.

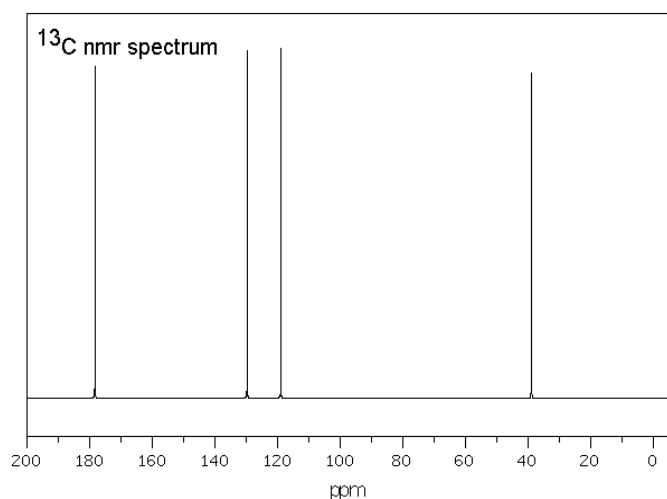
When performing this task, it is common to go through each piece of evidence to identify the parts of the molecule and to put them together. This can be a cyclical procedure with each spectrum analyzed at more than once.

Critical thinking questions

1. A compound has a strong absorption near 1720 cm^{-1} , but no absorptions above 3000 cm^{-1} in its infrared spectrum. It has a parent ion at m/z 86 in its mass spectrum and its ^{13}C NMR spectrum is given below. Give a structure consistent with these data.



2. A compound of molecular formula $C_4H_6O_2$ has strong absorptions in the infrared spectrum at 1670 cm^{-1} and 3400 cm^{-1} . The ^{13}C NMR spectrum is given below. Give a structure consistent with these data. If your answer is ambiguous, suggest a spectroscopic technique that could be used to resolve it.



3. A compound of molecular formula $C_9H_{10}O_2$ has a strong absorption in the ultraviolet spectrum around 265 nm , and strong absorptions in the infrared spectrum at 1670 cm^{-1} and 2900 cm^{-1} . The mass spectrum and ^{13}C NMR spectrum are given below. Give a structure consistent with these data.

