Structure determination

Learning objectives

1. Analyse and interpret infrared, 13C NMR and 1H NMR spectra
2. Suggest chemical structures based on spectral evidence

Activity

Below are the skeletal structures for 7 compounds.

Decide which set of spectra sets **A-G** from the following pages belong to each compound.

|  |  |  |
| --- | --- | --- |
| A picture containing hanger  Description automatically generatedethyl propanoate  **Spectra set \_\_\_\_\_** | Diagram  Description automatically generatedethanamide  **Spectra set \_\_\_\_\_** | A picture containing antenna, clock  Description automatically generated2-bromo-2-methyl propane  **Spectra set \_\_\_\_\_** |
| Diagram  Description automatically generatedbenzoic acid  **Spectra set \_\_\_\_\_** | Diagram  Description automatically generated2-hydroxybenzoic acid  **Spectra set \_\_\_\_\_** | A picture containing table  Description automatically generatedadamantane  **Spectra set \_\_\_\_\_** |
|  | A picture containing hanger, clock  Description automatically generated1,2-diacetoxyethane  **Spectra set \_\_\_\_\_** |  |

Before you begin read the **Helpful information** on the next page.

Make sure you have a data book or sheet available to help you identify key bonds and groups present.

Helpful information

1. In the 1H NMR the relative height of the red line shows the integration of each of the peaks. Where peaks are split a zoomed in section of the spectrum is given to show the splitting pattern.

Chart

Description automatically generated

1. These are real spectra so in some instances small peaks of impurities are seen.
2. You may also see peaks owing to the solvent used to dissolve the sample.

CDCl3 δC 77 ppm (three lines 1:1:1) and δH 7.25 ppm

DMSO δC 39.5 ppm (septet) and δH 2.50 ppm (quintet)

Chart

Description automatically generatedSpectra set A

Infrared

Chart, histogram

Description automatically generated

13C NMR

A picture containing chart

Description automatically generated

1H NMR

Chart

Description automatically generated with medium confidenceSpectra set B

Chart, line chart

Description automatically generatedChart

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Infrared  
  
  
  
  
  
  
  
  
  
  
  
  
  
  
13C NMR  
  
  
  
  
  
  
  
  
  
  
  
  
  
  
1H NMR

Chart

Description automatically generatedSpectra set C

Chart

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Infrared  
  
  
  
  
  
  
  
  
  
  
  
  
  
  
13C NMR  
  
  
  
  
  
  
  
  
  
  
  
  
  
  
1H NMR

Chart

Description automatically generatedSpectra set D

Graphical user interface, application, table, Excel

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Infrared  
  
  
  
  
  
  
  
  
  
  
  
  
  
  
13C NMR  
  
  
  
  
  
  
  
  
  
  
  
  
  
  
  
1H NMR

Chart

Description automatically generatedSpectra set E

Chart, line chart

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Infrared  
  
  
  
  
  
  
  
  
  
  
  
  
  
  
Chart, line chart

Description automatically generated13C NMR  
  
  
  
  
  
  
  
  
  
  
  
  
  
  
1H NMR

A picture containing graphical user interface

Description automatically generatedSpectra set F

Chart

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Chart

Description automatically generated13C NMR  
  
  
  
  
  
  
  
  
  
  
  
  
  
  
1H NMR

Chart

Description automatically generatedSpectra set G

Chart

Description automatically generatedChart

Description automatically generated  
  
  
  
  
Infrared  
  
  
  
  
  
  
  
  
  
  
  
  
  
  
13C NMR  
  
  
  
  
  
  
  
  
  
  
  
  
  
  
1H NMR