Structure determination

Learning objective

- 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.

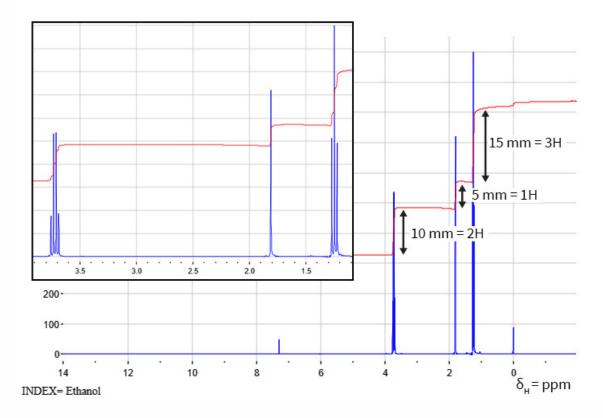
ethyl propanoate	ethanamide	2-bromo-2-methyl
		propane
0		
	NH ₂	 Br
	2	
Spectra set	Spectra set	Spectra set
benzoic acid	2-hydroxybenzoic acid	adamantane
0		
ОН	ОН	
	ОН	
Spectra set	Spectra set	Spectra set
	1,2-diacetoxyethane	
	O	
	0	
	Spectra set	

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.



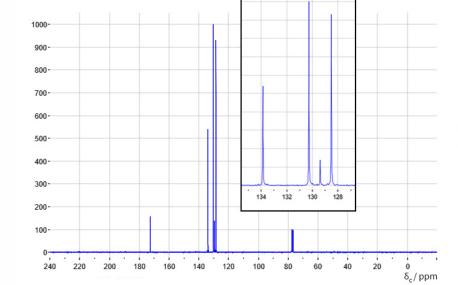
- 2. These are real spectra so in some instances small peaks of impurities are seen.
- 3. You may also see peaks owing to the solvent used to dissolve the sample. $CDCl_3 \delta_C$ 77 ppm (three lines 1:1:1) and δ_H 7.25 ppm DMSO δ_C 39.5 ppm (septet) and δ_H 2.50 ppm (quintet)

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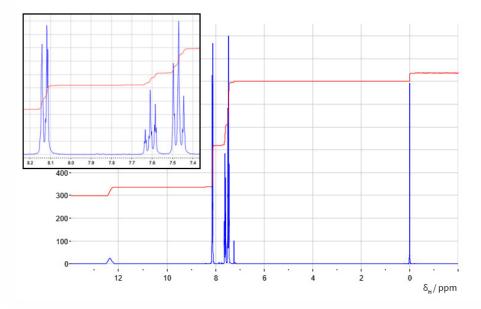
Spectra set A

Infrared

97.5 92.5-87.5-82.5-77.5-72.5-62.5-52.5 42.5-37.5-1000 2000 3500 3000 2500 1500 4000 Wavenumber / cm⁻¹



¹H NMR



13C NMR

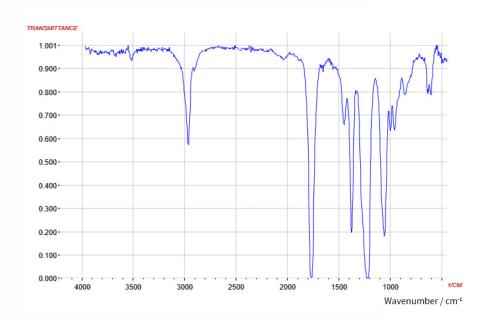
Education in Chemistry 16–18 years

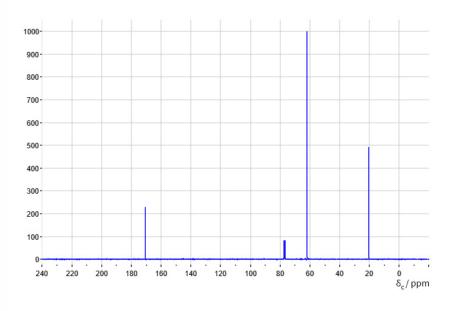
Downloaded from https://rsc.li/3FwsQjf

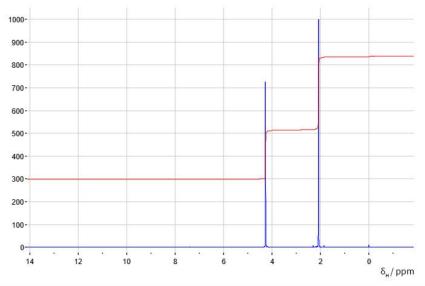
Spectra set B

Infrared

13C NMR







ARBITRARY UNITS 1100-1000-900-800-700-

600-

100-

Education in Chemistry 16–18 years

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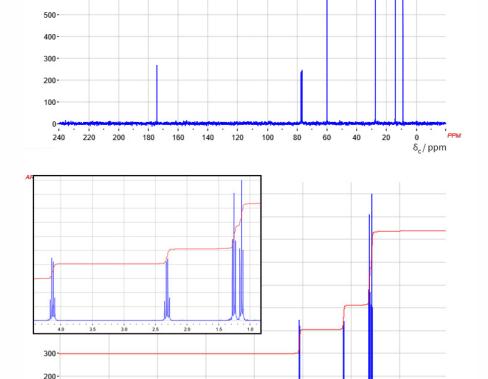
 $\delta^{}_{_{\text{H}}}/\,\text{ppm}$

Spectra set C

Infrared

TRANSMITTANCE 100 90-80-60-40-20-10-0า 4000 3000 3500 2500 2000 1500 1000 Wavenumber / cm⁻¹

13C NMR



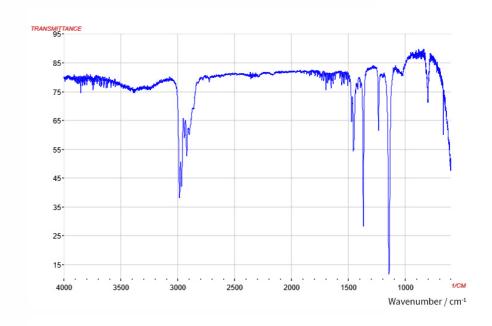
Education in Chemistry 16–18 years

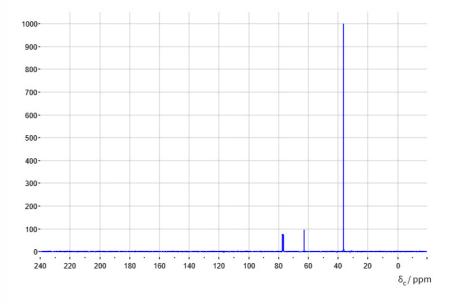
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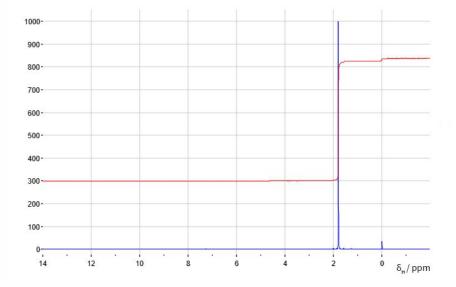
Spectra set D

Infrared

¹³C NMR





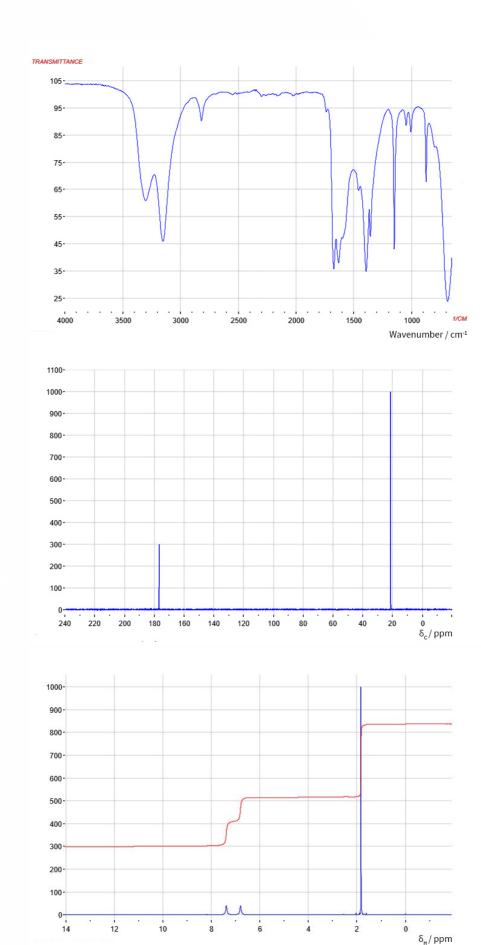


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Spectra set E

Infrared

¹³C NMR



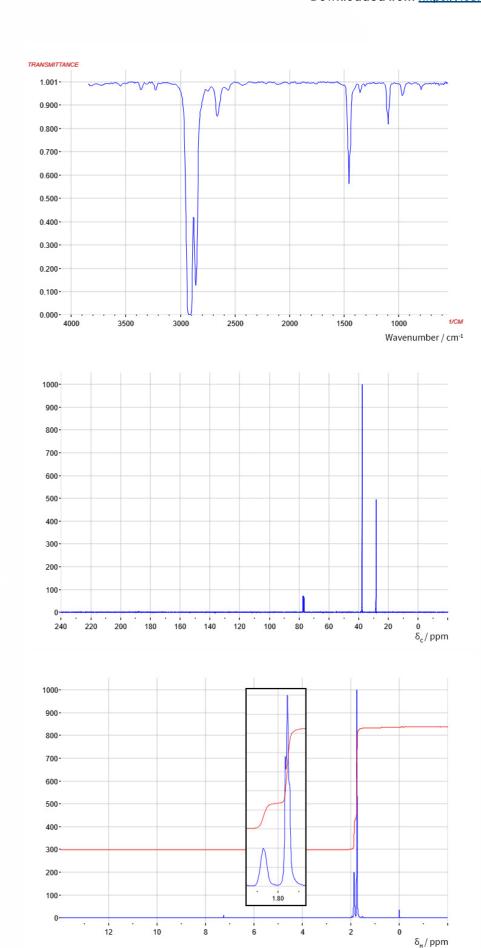
Education in Chemistry 16–18 years

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Spectra set F

Infrared

¹³C NMR



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Spectra set G

Infrared

¹³C NMR

