Structure determination

This resource accompanies the article **How to teach structure determination** in *Education in Chemistry* which can be viewed at: https://rsc.li/3FwsQjf

Learning objectives

1 Apply an understanding of infrared, ^{13}C NMR and ^{1}H NMR spectra

2 Identify the spectra of given compounds

Introduction

Test learners' ability to suggest chemical structures based on spectral evidence by asking them to match the skeletal structures in the student worksheet to the sets of infrared, ^{13}C and ^{1}H NMR spectra.

Notes

If learners struggle to get started with this activity, encourage them to pick one molecule and identify key features they would expect to see in the spectra such as:

- Strong absorbances (C=O, O-H) in the infra-red spectra
- Number of peaks in the ^{13}C NMR spectrum and approximate chemical shifts

This will enable learners to narrow down the number of possible matches before looking at the now reduced number of spectra in more detail.

Full interpretation of spectra is not necessary to complete the activity but would provide a suitable challenge and help learners develop mastery in structure determination.

Answers

Spectra set A: benzoic acid

Spectra set B: 1,2-diacetoxyethane

Spectra set C: ethyl propanoate

Spectra set D: 2-bromo-2-methyl propane

Spectra set E: ethanamide

Spectra set F: adamantane

Spectra set G: 2-hydroxybenzoic acid