**Raffles Institution**
**Year 6 H3 Chemistry 2025**

**Tutorial 5B: Structural Elucidation using Mass Spectrometry, IR Spectroscopy and NMR Spectroscopy**

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**Use the following table to work out and tabulate your data for the questions in the tutorial.**

**NMR spectrum**

| δ/ppm | Integration | Splitting | Deductions |
|---|---|---|---|
| | | | |
| | | | |
| | | | |

**IR spectrum**

| Wavenumber ($cm^{-1}$) | Deductions |
|---|---|
| | |
| | |

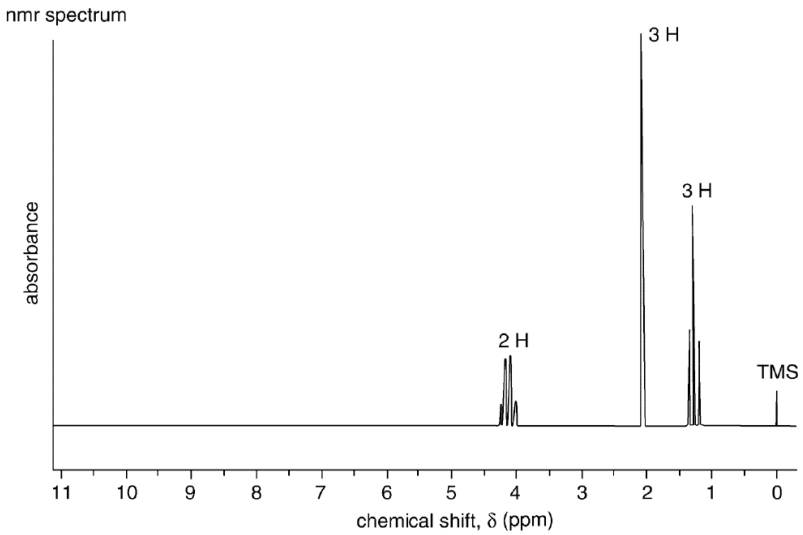
**Mass spectrum**

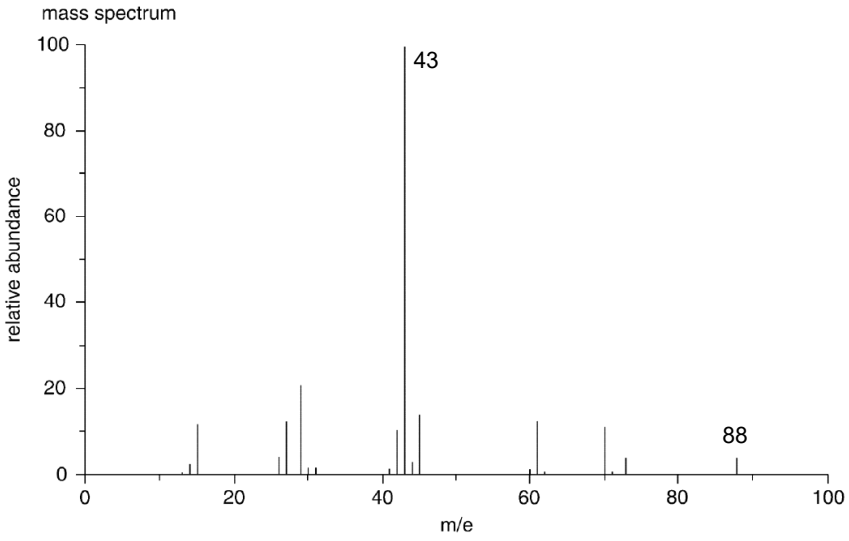
| m/e | Species responsible / Deductions |
|---|---|
| | |
| | |

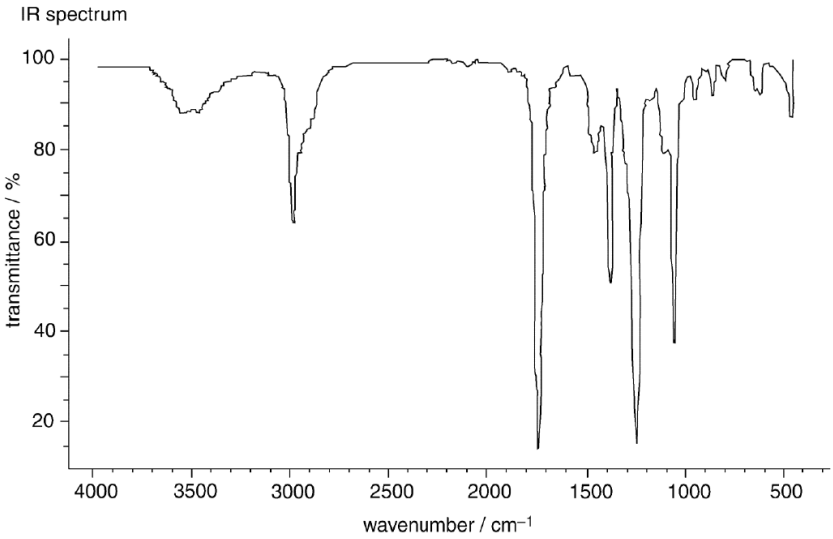
**Self-Check Question** *(refer to IVY for solutions to self-check questions)*

**Q1** Interpret the following spectra and use them to suggest a structure for compounds **A** and **B**.

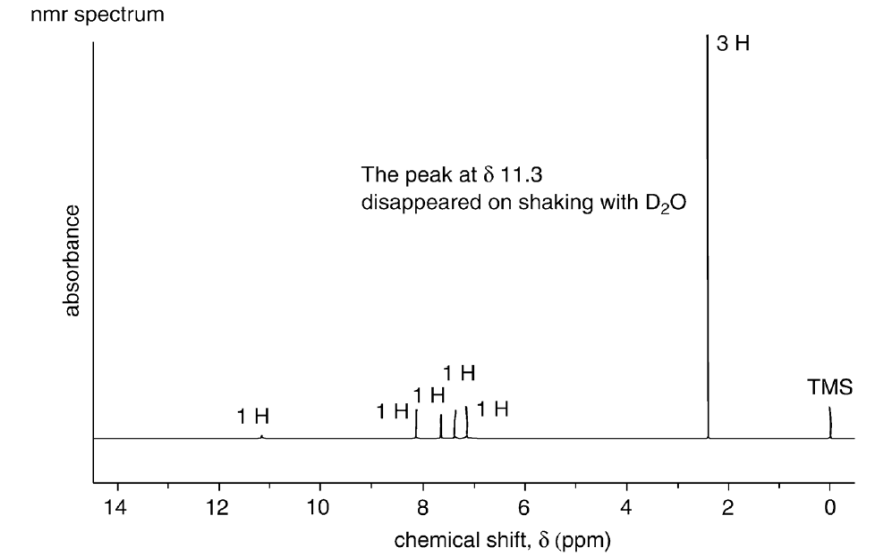
**(a) Spectra for compound A**

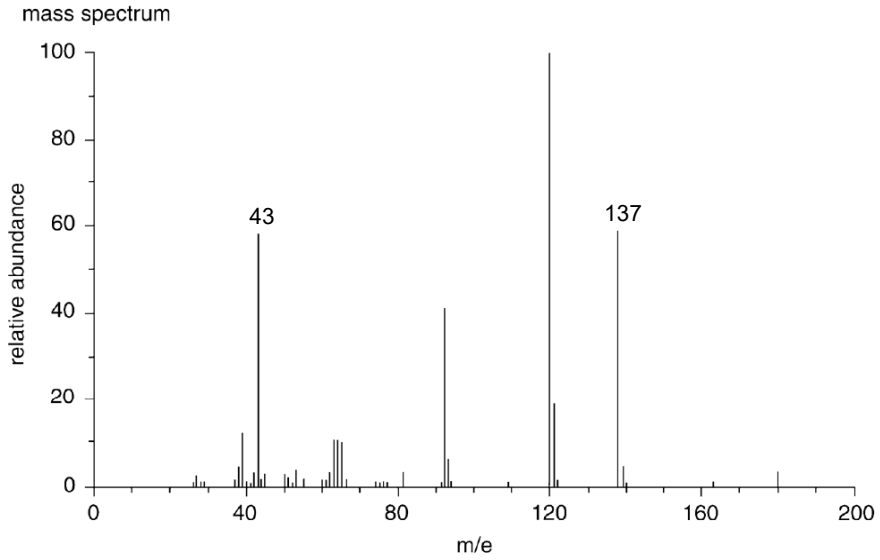


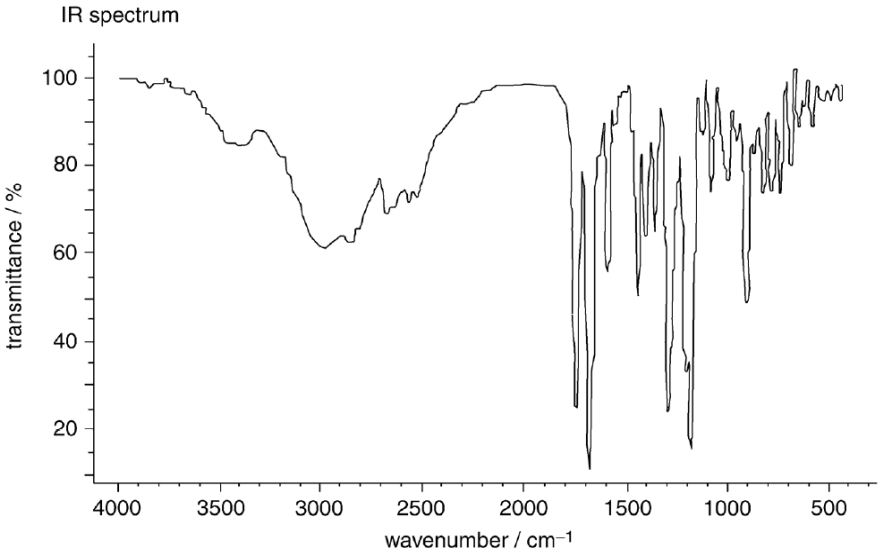



**(b) Spectra for compound B**



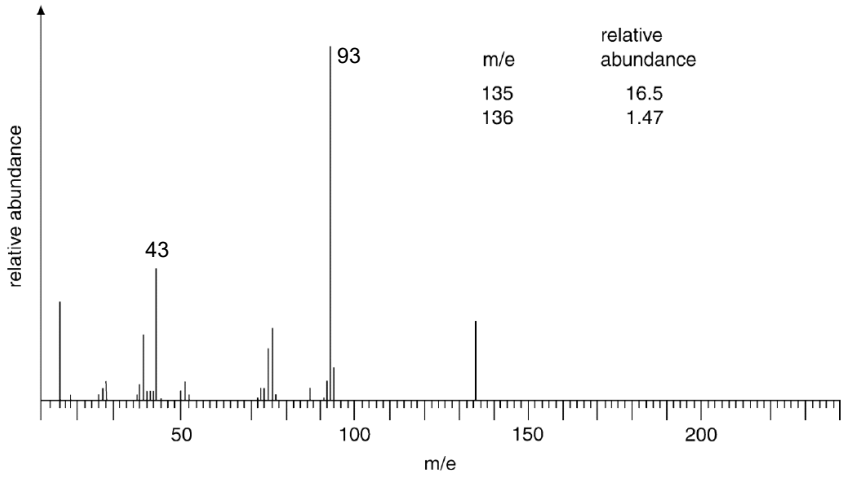



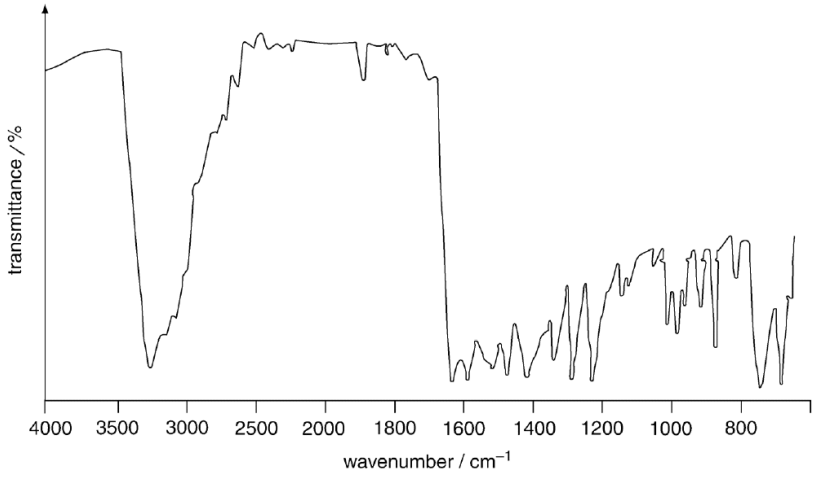



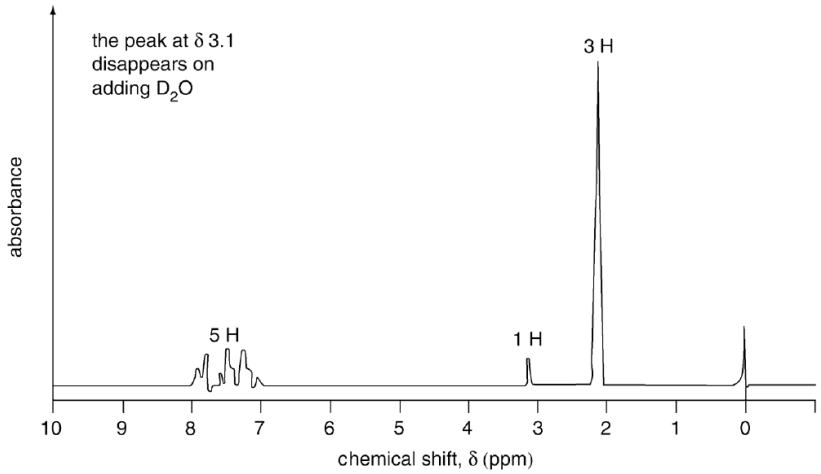
## Practice Questions

### Q2

The spectra shown below were obtained from compound Q, which contains the elements carbon, hydrogen, nitrogen and oxygen.



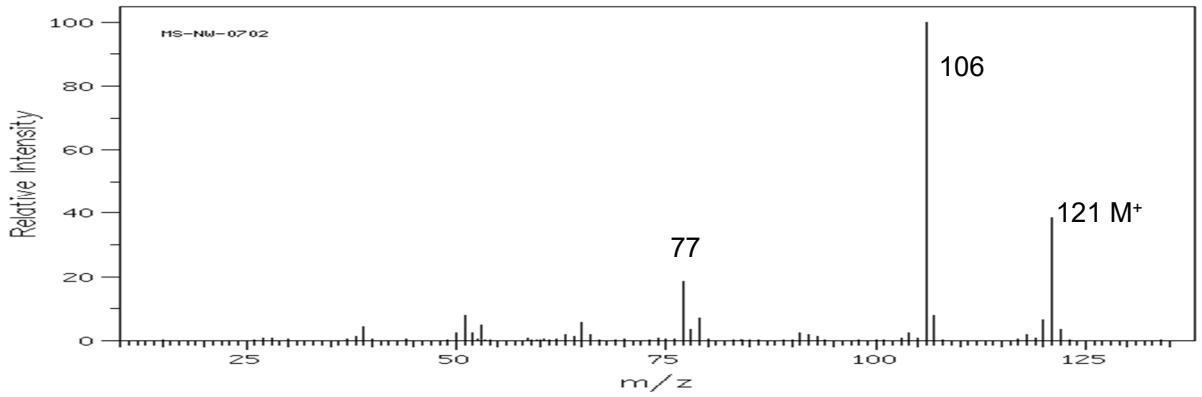



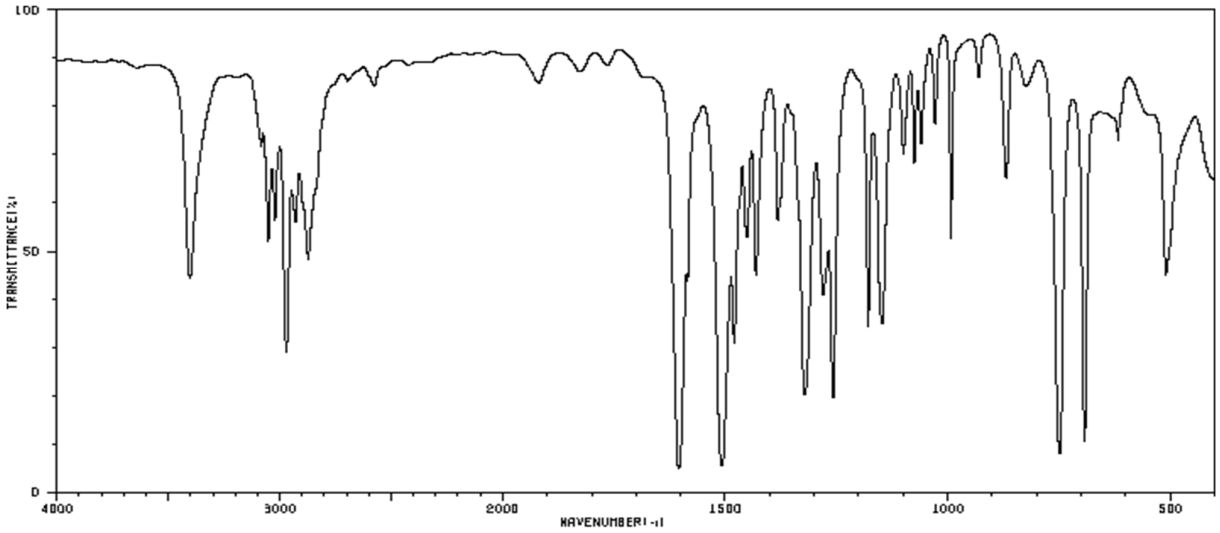

(a) Consider the nmr, mass and ir spectra in turn. Explain what information each spectrum gives about the structure of Q.

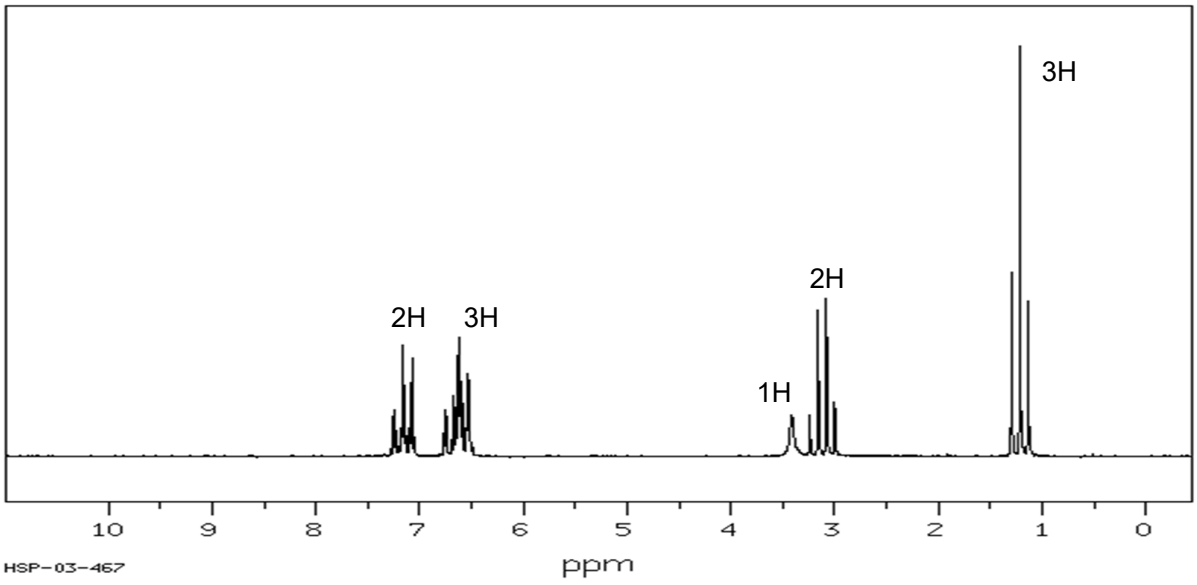
(b) Use your answer to (a) to suggest what functional groups are present in Q and hence give a possible structure for the compound.

**Q3**
Interpret the following spectra and use them to suggest a structure for compounds **1** and **2**.

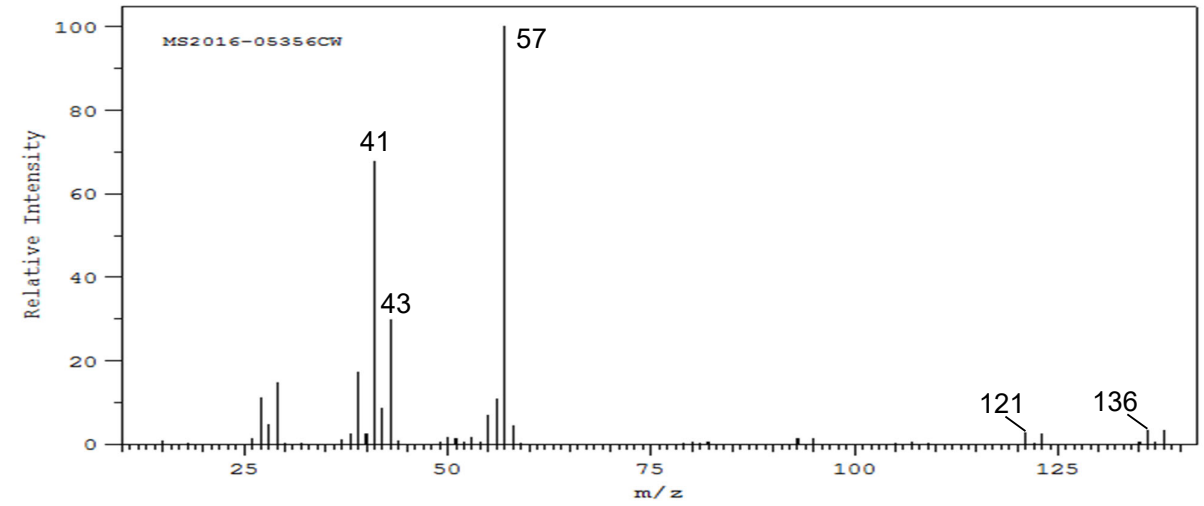
**(a) Spectra for compound 1**

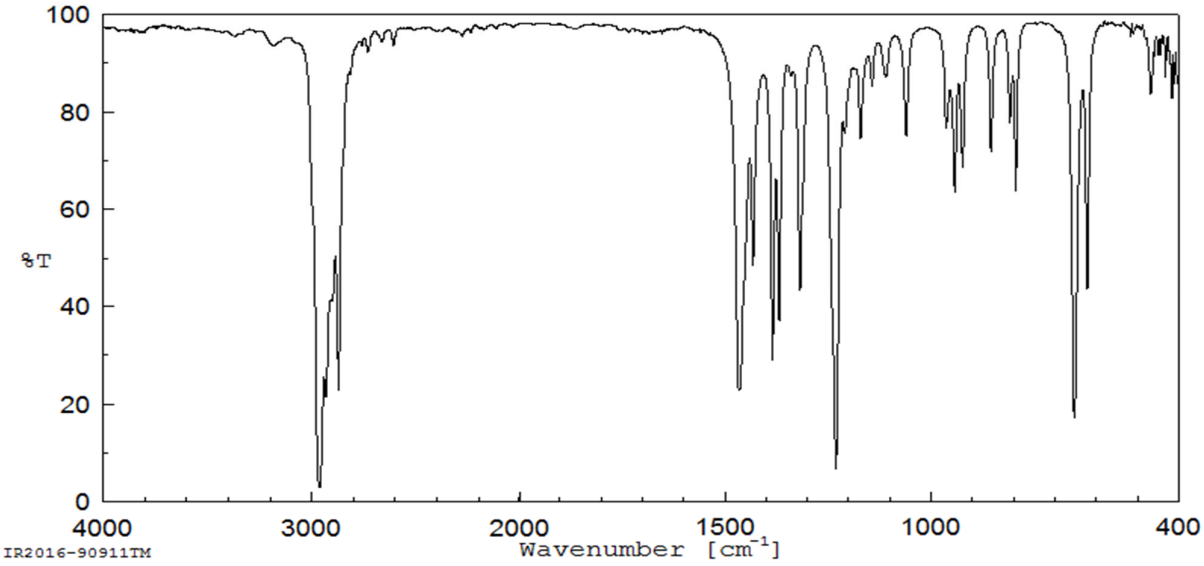


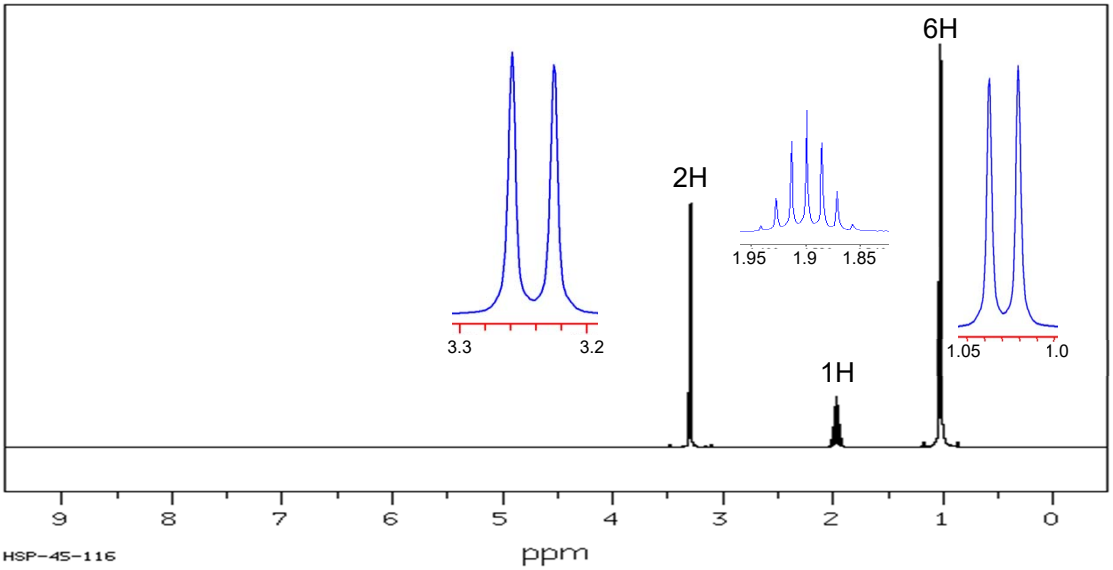



**(b) Spectra for compound 2**

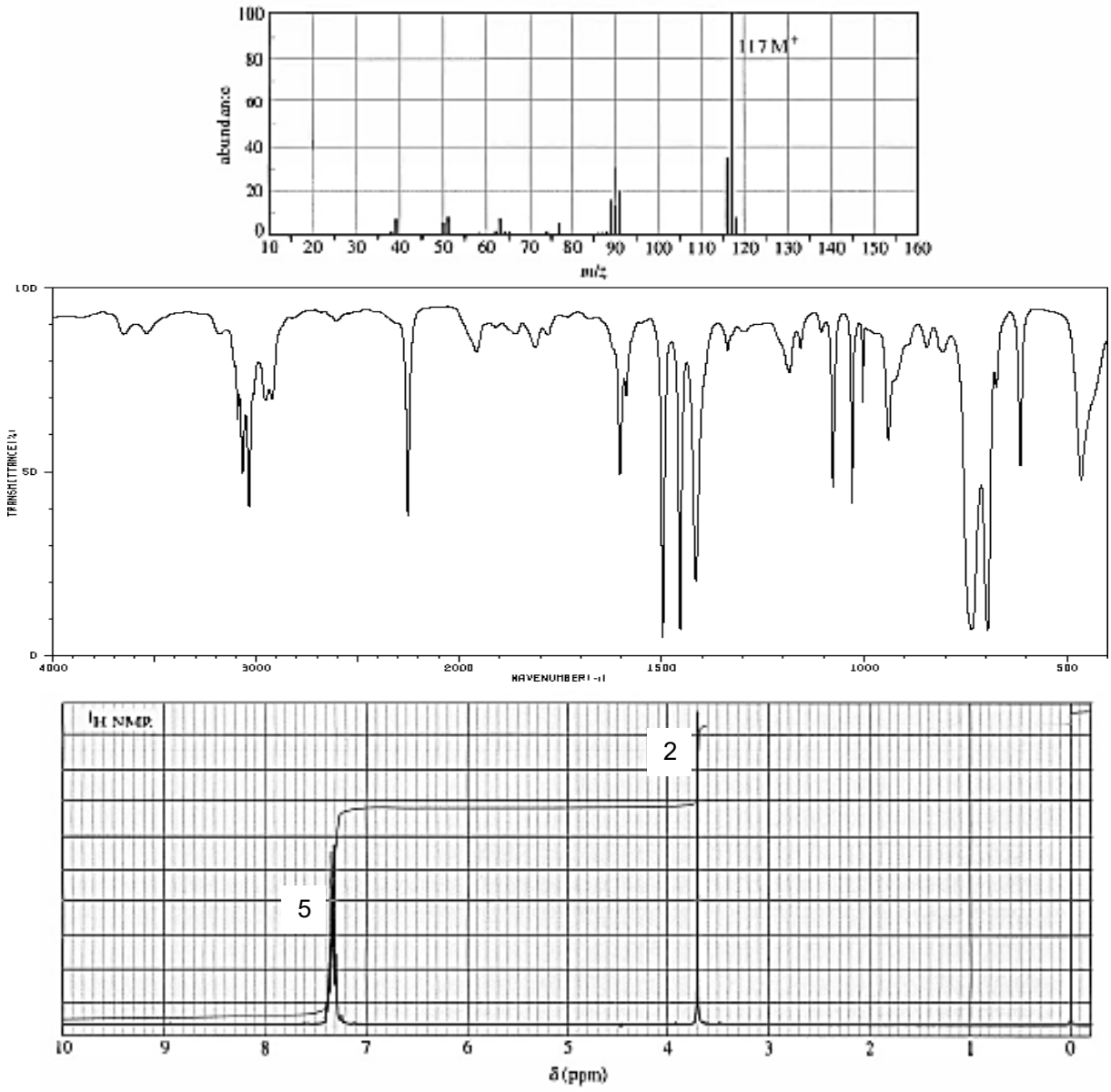


**Q4**

A compound **X** was isolated as a minor constituent in an extract from garden cress. Its spectra are shown below. Interpret the spectra given and suggest a structural formula for **X** showing reasoning.



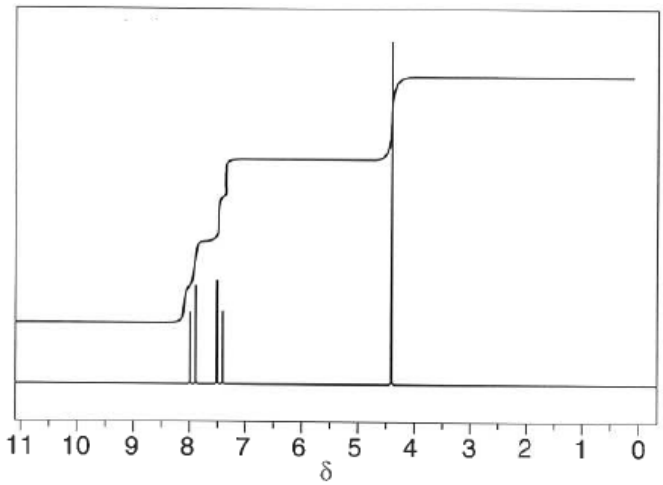
**Q5 [N12/4(b)]**

Compound **H** is a useful intermediate for the synthesis of drugs. Apart from carbon, hydrogen and oxygen atoms, the molecule **H** contains at least two halogen atoms, which may be chlorine or bromine of a mixture of both.

The major peaks in its mass spectrum are listed in the table below

| m/e value | % abundance |
|---|---|
| 75 | 14.7 |
| 111 | 25.7 |
| 113 | 8.7 |
| 139 | 100.0 |
| 141 | 34.7 |
| 232 | 5.7 |
| 234 | 7.6 |
| 236 | 1.9 |

The NMR spectrum of **H** is shown below. Relative number of protons responsible for each NMR signal may be inferred from the integration trace shown on the spectrum.




**(i)** Use the mass spectrum to determine the number of atoms of each halogen contained in the molecule of **H.**

**(ii)** Analyse the NMR spectrum to suggest the likely environments of the protons in the molecule of **H**, and the number of protons in each environment.

**(iii)** Apart from the molecular ion peaks, identify which of the peaks in the mass spectrum arise from fragments that contain bromine or chlorine atoms, and suggest which halogen they contain.

**(iv)** Suggest the molecular formulae of the fragments responsible for the peaks in the mass spectrum.

**(v)** Use the information you have derived from the two spectra to suggest a structure for **H**