

Spectra

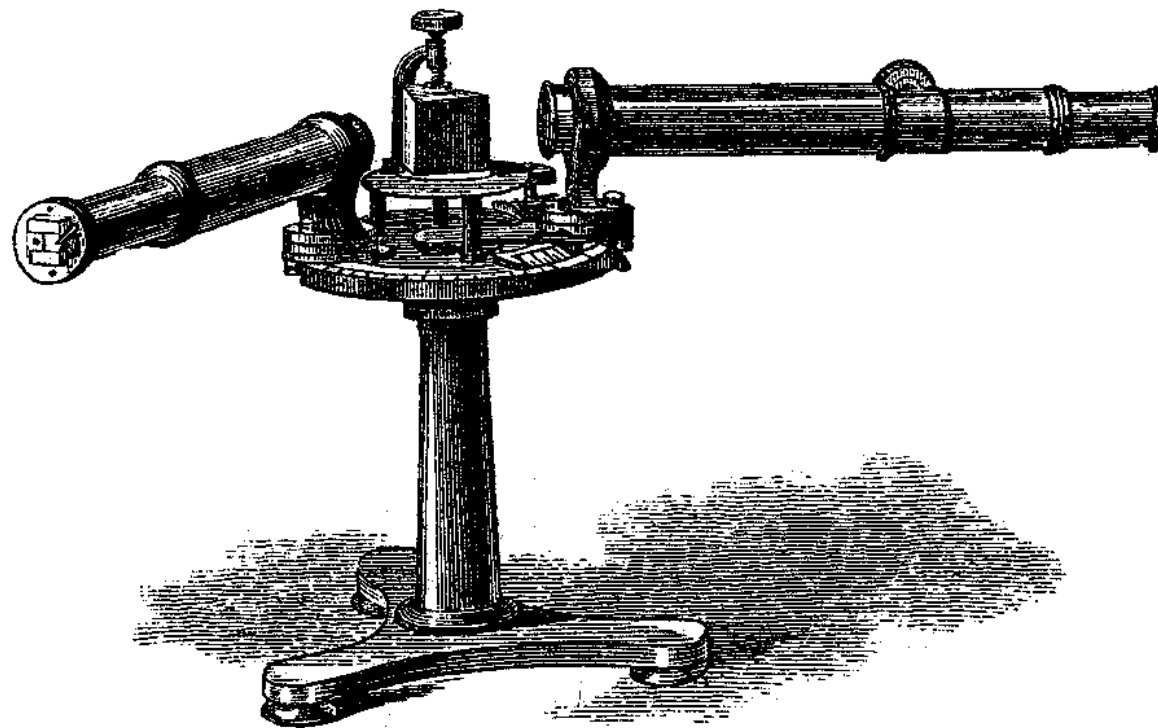
L202

September 2000

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Spectra



SCHOOL SCIENCE SERVICE

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We would like to thank the Aldrich Chemical Company for supplying many of the spectra and Dr. Kikuko Hayamizu of the National Institute of Materials and Chemical Research (NIMC) in Japan for allowing us to use material from the web site www.aist.go.jp.

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Guide L202

Spectra

1 The scope of this guide

This is a new edition of the 1993 guide. Not only does it contain the infra-red (ir) and mass spectra of 40 common organic compounds but also the ^{13}C and ^1H nuclear magnetic resonance spectra (nmr). Where available, there is also information about the ultra-violet (uv) spectra. The spectra are suitable for use by students and teachers in post-GCSE chemistry courses. Compared to the former edition of L202, the spectra of some further chemicals have been introduced while a few have been removed.

Before spectroscopy was commercially available, identification of an unknown substance required breaking it down chemically into its constituent elements to find the empirical formula and using specific reactions to elucidate the structure. This was a time-consuming and often inaccurate procedure. Spectroscopy has shortened greatly the time required for the accurate determination of molecular structures.

Structure determination using spectroscopy is included in a number of A-level courses¹ either in the core or as a special study. Some science departments may have an old ir or uv-machine given to them by a local firm or university but maintenance and finding spares can raise problems. A mass

spectrometer requires high vacuum techniques and nmr spectroscopy involves special solvents and high magnetic fields; neither of these is available in most schools. However, it is well worth organising a visit to see these machines in action at a local university or research laboratory.

It should be made clear to students the difference in the nature of these spectra. Ir, uv and nmr spectra involve the absorption of electromagnetic radiation. However, a mass spectrum shows a range of masses of molecular fragments caused by bombarding molecules with electrons. The important factor is that each chemical has its own “fingerprint” of spectra by which it can be identified.

If you wish to download spectra of other chemicals, then the site www.aist.go.jp can be used. In providing you with this information, we trust that you will not contravene the restrictions that the keepers of the site impose.

2 How to use the guide

The published spectra may be photocopied for use with students. The names of the substances are not printed on the sheets so that they can be used as unknowns if required; a list can be found on page 6.

The examples of spectra in this guide may be used in several ways.

¹ For example, Edexcel Advanced GCE, Chemistry (Nuffield), Topics 20 and 21.

- When molecular structure determination is introduced within the syllabus, the spectra may be used as examples.
- A discussion of structural isomerism can be enhanced by pointing out that, although the chemical analyses of isomers are the same, the "chemical fingerprint", shown by spectra, differs from one isomer to another.
- During practical lessons, the spectra of the reacting chemicals may be compared to that of the product.
- The spectra can be used as problem-solving exercises.

The layout of the pages of spectra is shown in Figure 1.

Reference number of substance	Ultra-violet spectrum	Analysis
This can be compared with the index on page 6	If results are available, the wavelength (in nm) and absorption coefficient are given.	The percentage by mass of the elements in each substance is given.
Infra-red spectrum By reference to the infra-red correlation chart (see Appendix 1), functional groups within the molecule can be identified.	¹H magnetic resonance spectrum The chemical shift (δ) at which the absorption takes place can be compared with the correlation charts provided (see Appendix 2). Although the peaks, depending on their molecular environment, may be split into doublets, triplets, quartets and even more complicated patterns, students are not expected to interpret this information.	
¹³C magnetic resonance spectrum The chemical shift (δ) at which the absorption takes place can be compared with the correlation charts provided (see Appendix 3). Although the peaks, depending on their molecular environment, may be split into doublets, triplets, quartets and even more complicated patterns, students are not expected to interpret this information.	Mass spectrum The fragments flagged with their mass numbers represent those that can either be easily identified from the simple fragmentation of the molecular ion or are fragments from rearrangement reactions that are of diagnostic value (section 6). Any other peaks formed from rearrangement reactions are beyond the scope of A-level courses. The value of the molecular ion is always given even if the intensity of the signal is low.	

Figure 1 Layout of the spectra (see section 7)

3 Ultra-violet spectra

The ultra-violet region of the spectrum has a wavelength of between 200 and 400 nm. In this region, outer electrons in certain areas of a molecule are promoted to higher energy states. Absorption usually indicates unsaturation in the molecule, eg, arenes, alkenes and carbonyl groups. Where molecules exhibit a high degree of conjugation, the absorption of energy takes place in the visible region (400 - 800 nm) of the spectrum and substances appear coloured, eg, dyes. If values in the literature are available, the wavelength (λ) at which absorption takes place, along with the absorption coefficient (ϵ), are given. Uv-spectra are more often used to measure concentration than to determine molecular structure. However, as this form of spectroscopy is mentioned in the syllabuses, the values, where available, are included.

4 Infra-red spectra

The infra-red wavelength region of the electromagnetic spectrum ranges from 800 to 2500 nm. It is traditional to express this as a "wavenumber" which is the reciprocal of the wavelength in centimetres, ie, 13333 to 400 cm⁻¹. The region between 4000 and 660 cm⁻¹ is of particular interest to the organic chemist. Absorption bands in this region result from the energy absorbed when the molecule bends and stretches. The energy required to bend or stretch a bond is not affected by structural arrangements in other areas of a molecule but structural changes close to the vibrating bond can cause small shifts in the value of the wavenumber. For example, all carbonyl (C=O) stretching vibrations occur between 1680 and 1795 cm⁻¹ but the carbonyl group in alkyl carboxylic acids

absorbs energy between 1700 and 1725 cm^{-1} whereas in aryl carboxylic acids it absorbs between 1680 and 1700 cm^{-1} . Hence, an infra-red spectrum is useful in identifying functional groups and in giving some idea of the molecular environment. Appendix 1 is a correlation chart relating the energy at which absorption takes place for particular functional groups.

5 Nuclear magnetic resonance spectroscopy

The property of “spin” not only applies to electrons but also to protons and neutrons. These particles act as tiny bar magnets and if there is an odd number of particles present, as in ^1H and ^{13}C , the application of a large external magnetic field can induce a separation of energy levels in the nuclei. By application of external radiation at precise energy levels, nuclei can be promoted from the lower energy to the higher level. The energy at which this occurs can be measured and usually falls within the radiowaves of the electromagnetic spectrum. The chemical shift (δ) compares this absorbed energy to that of a standard substance: tetramethylsilane. The value of the chemical shift depends on the electron environment of the nucleus. So if a ^{13}C or a ^1H atom is attached to a carbonyl group, this will produce a signal at a different energy to that of these atoms on a benzene ring or a methyl group. The functional group in which these atoms are involved can therefore be identified. The signals are sometimes split into doublets, triplets etc and even more complicated patterns. These also have diagnostic value. The chemical shift and patterns can also be influenced by temperature, solvent and concentration, especially where inter- and intra-hydrogen bonding occurs (eg, salicylic acid). Trichloromethane-*d*, the deuterated form of

trichloromethane, is used as the solvent for the spectra in section 7.

As ^1H atoms are plentiful in nature but ^{13}C atoms are rare, ^1H nmr spectroscopy was developed before ^{13}C nmr spectroscopy. However, the latter is now widely used and ^{13}C spectra are included in this guide to bring students up to date with modern developments. Appendices 2 and 3 show the correlation of the chemical shifts with various functional groups.

6 Mass spectra

In the mass spectrometer, a molecule is bombarded with high-energy electrons which remove an electron from the molecule to produce a positive molecular ion² (also called the parent ion). Such ions are accelerated through a magnetic field towards the detector. However, before these ions reach the detector, some will fragment and/or rearrange into ions with a range of mass-to-charge (m/z) values up to that of the parent ion. This is called a fragmentation pattern but is often called a “mass spec”. Both the precise value of the mass of the molecular ion and the fragmentation pattern are of diagnostic value.

6.1 The molecular ion

The accurate relative molecular mass of a molecule, found using high-resolution mass spectrometry, is used to identify the chemical composition of a substance. Methanal (CH_2O)

2 More than one electron can be removed but the interpretation of these results is not required for Advanced-level work.

and ethane (C₂H₆) both have an integral relative molecular mass of 30 but, using the values in Table 1, the accurate masses would be 30.010565 and 30.046950 respectively and hence correct identification of the formula is possible.

Table 1 Accurate relative atomic masses

Isotopes	Atomic mass
Hydrogen	1.00782506
Carbon	12.00000000
Nitrogen	14.00307407
Oxygen	15.99491475
Chlorine	34.96885300
Bromine	78.91833200

The intensity of molecular ions can vary between very strong and weak depending on the stability of the ion as it passes through the magnetic field. If the molecular ion is very unstable, it fragments into smaller ions and very few molecular ions will reach the detector, producing a weak signal. Whether the intensity of the molecular ion is strong or weak is shown in Table 2.

Table 2 Intensity of the molecular ion

Strong	Medium	Weak
Aromatic hydrocarbons, aromatic amines and cyclic compounds.	Benzoyl and benzyl compounds, straight chain ketones, aldehydes, acids, esters, ethers and alkyl halides.	Branched chain compounds, aliphatic alcohols and amines.

Where the intensity of the molecular ions is weak, in the published spectra, the mass of the ion is still given along with

the magnification required to view the peak (eg, see Substance 1, 2-aminopropanoic acid).

6.2 Isotopes

Molecular ions containing chlorine (75% ³⁵Cl and 25% ³⁷Cl) or bromine (50% ⁷⁹Br and 50% ⁸¹Br), will produce more than one parent-ion peak depending on the abundance of each isotope and the number of such atoms in the original molecule. The characteristic patterns of these parent ions are shown in Figure 2.

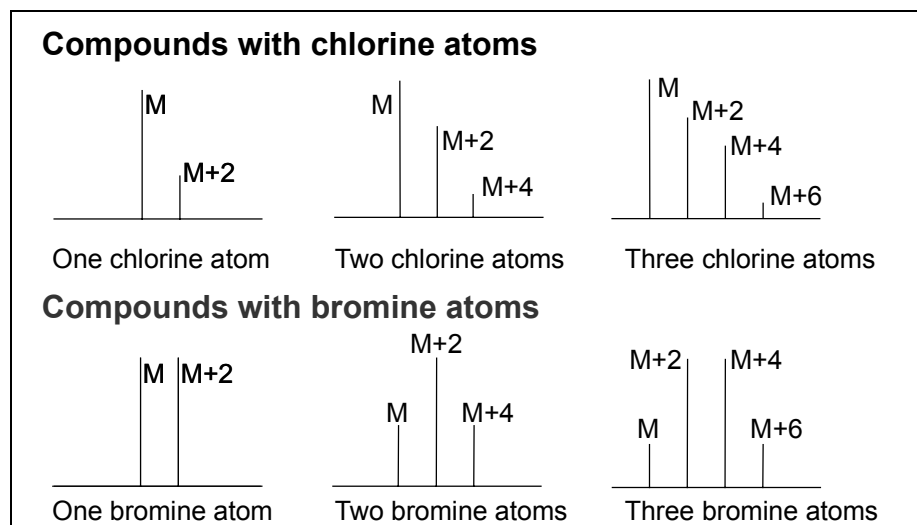


Figure 2 Effect of isotopes on the molecular ion

6.3 Fragmentation patterns

Molecular ions fragment in the mass spectrometer to give a diagnostic pattern for each particular substance. The process is summarised in Figure 3.

The molecule ABCD forms a molecular ion which then fragments into smaller ions (all shown in **bold** print) with lower mass numbers. These ions may also have enough energy to fragment into smaller ions.

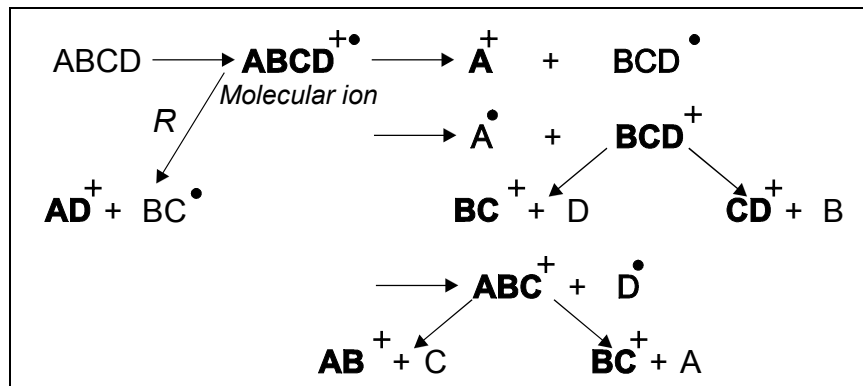


Figure 3 How fragmentation occurs

Reaction "R" represents one of a large number of rearrangement reactions that can occur. (Other rearrangements would produce AC^+ or BD^+ ions.) These give rise to mass values which appear to bear no resemblance to the original molecule, although they may be of diagnostic value. Identification of these reactions comes with experience and these peaks are not flagged with their mass values in the published spectra except those to which reference is made in Tables 3 and 4.

For example, in substance 2, (benzoic acid, C_6H_5COOH), the values of the mass-to-charge (m/z) ratios, ie, 122, 105, 78, 77, 51 and 50, are quoted but not that at 28. The peak at 122 is caused by the molecular ion, $C_6H_5COOH^+$, and the peaks at 105 ($C_6H_5CO^+$) and 77 ($C_6H_5^+$) can be explained by the fragmentation of the molecular ion. The peaks at 50, 51 78 and 79 are common to substituted aromatic compounds (see Table 3).

Substance 27, methyl benzoate, shows a peak at 105 which is 31 less than the molecular ion at 136 (ie, $M - 31$). This loss of 31 is indicative of the removal of the $-OCH_3$ group as shown in Table 4.

Table 3 Diagnostic mass numbers which indicate a particular functional group

Mass-to-charge (m/z) ratio	Possible inference
44	Aldehydes or amides
45	Alcohols
50, 51, 78, 79	Phenyl group

Table 4 Characteristic masses caused by the loss of a fragment from a parent ion

Mass-to-charge (m/z) ratio	Possible inference
$M - 15$	Loss of a $-CH_3$ group
$M - 18$	Loss of water from an alcohol
$M - 29$	Loss of a $-C_2H_5$ group
$M - 31$	Loss of a $-OCH_3$ group
$M - 36$	Loss of hydrogen chloride from a primary halide
$M - 42$	Loss of CH_2CO from aromatic ethanoates or amides
$M - 60$	Loss of ethanoic acid from ethanoates

7 The spectra

The following page gives a list of the chemicals for which spectra are included. The names of the chemicals are not provided on the spectra so that they can be used as problem-solving exercises. The spectra are given on the subsequent pages.

7.1 Index of spectra

	Substance	Molecular formula	Relative molecular mass (M_r)
1.	2-Aminopropanoic acid (alanine)	$C_3H_7O_2N$	89
2.	Benzenecarboxylic acid (benzoic acid)	$C_7H_6O_2$	122
3.	Butanal	C_4H_8O	72
4.	Butan-1-ol	$C_4H_{10}O$	74
5.	Butan-2-ol	$C_4H_{10}O$	74
6.	Butanone	C_4H_8O	72
7.	Butylamine	$C_4H_{11}N$	72
8.	1-Chlorobutane	C_4H_9Cl	92.5
9.	2-Chlorobutane	C_4H_9Cl	92.5
10.	1-Chloro-2-methylpropane	C_4H_9Cl	92.5
11.	2-Chloro-2-methylpropane	C_4H_9Cl	92.5
12.	Cyclohexane	C_6H_{12}	84
13.	Cyclohexanol	$C_6H_{12}O$	100
14.	Cyclohexene	C_6H_{10}	82
15.	Ethanamide	C_2H_5ON	59
16.	Ethanoic acid	$C_2H_4O_2$	60
17.	Ethanoic anhydride	$C_4H_6O_3$	102
18.	Ethanol	C_2H_6O	46
19.	Ethanoyl chloride	C_2H_3OCl	78.5
20.	2-Ethanoylbenzenecarboxylic acid (aspirin)	$C_9H_8O_4$	180

	Substance	Molecular formula	Relative molecular mass (M_r)
21.	Ethyl ethanoate	$C_4H_8O_2$	88
22.	Ethylamine	C_2H_7N	45
23.	Hexane	C_6H_{14}	86
24.	2-Hydroxybenzenecarboxylic acid (salicylic acid)	$C_7H_6O_3$	138
25.	2-Hydroxypropanoic acid (lactic acid)	$C_3H_6O_3$	90
26.	Limonene	$C_{10}H_{16}$	136
27.	Methyl benzoate	$C_8H_8O_2$	136
28.	Methyl 3-nitrobenzoate	$C_8H_7O_4N$	181
29.	Methyl propanoate	$C_4H_8O_2$	88
30.	2-Methylpropan-1-ol	$C_4H_{10}O$	74
31.	2-Methylpropan-2-ol	$C_4H_{10}O$	74
32.	Phenol	C_6H_6O	94
33.	Phenylamine	C_6H_7N	93
34.	n-Phenylethanamide (acetanilide)	C_8H_9ON	135
35.	Phenyl ethanoate	$C_8H_8O_2$	136
36.	Phenylethene (styrene)	C_8H_8	104
37.	Propanal	C_3H_6O	58
38.	Propan-1-ol	C_3H_8O	60
39.	Propan-2-ol	C_3H_8O	60
40.	Propanone	C_3H_6O	58

Substance 1

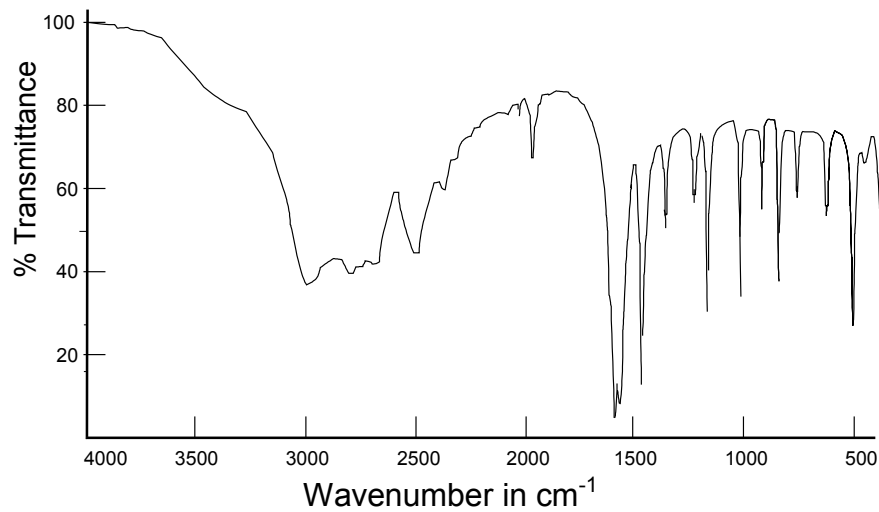
Ultra-violet spectrum

$\lambda = 205 \text{ nm}$, $\epsilon = 5$

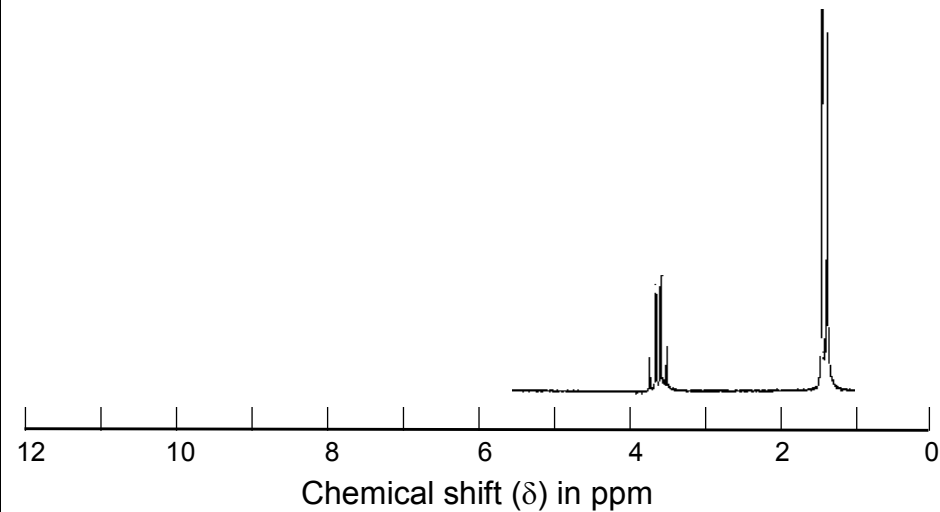
Analysis

Carbon	40.4%	Oxygen	36.0%
Hydrogen	7.9%	Nitrogen	15.7%

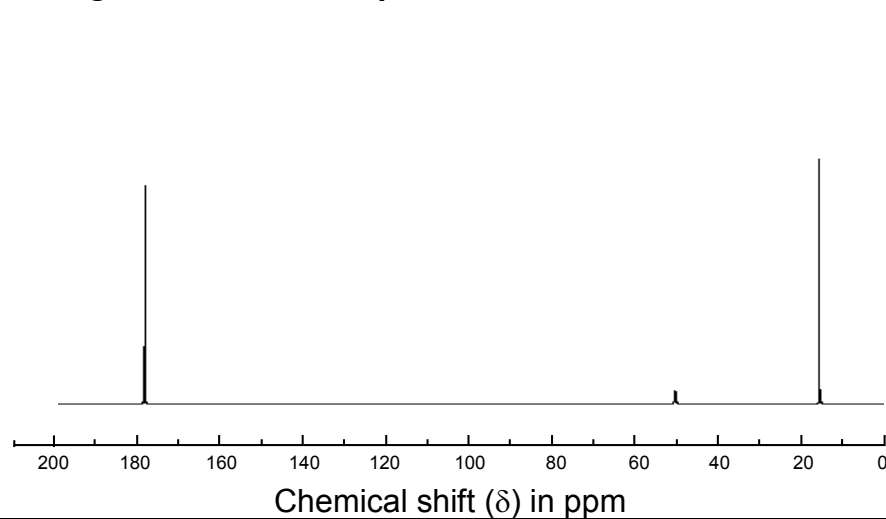
Infra-red spectrum



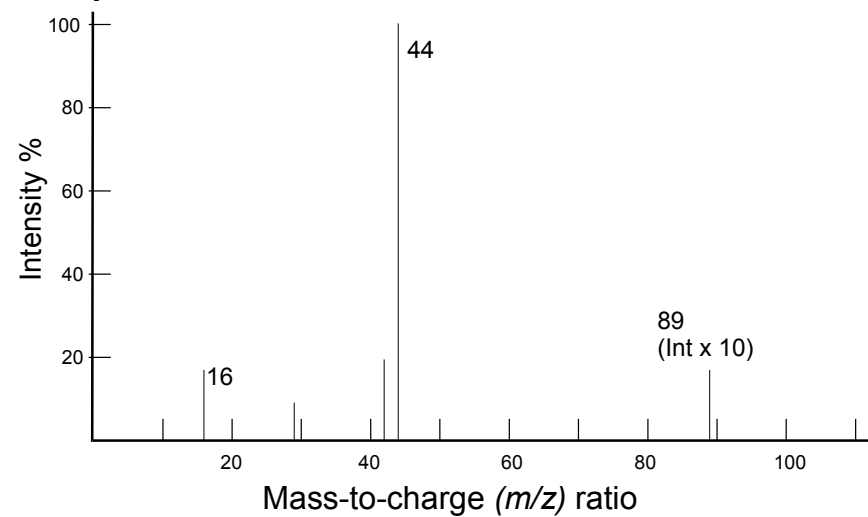
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 2

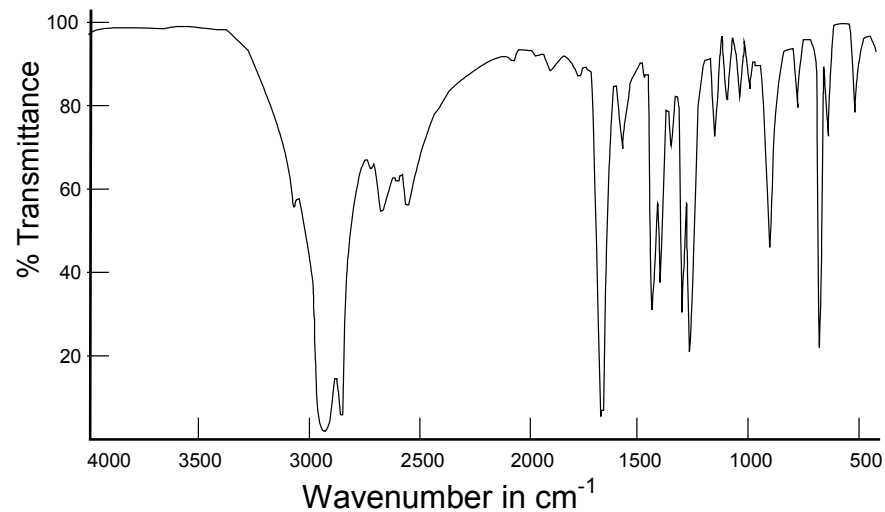
Ultra-violet spectrum

$\lambda = 228 \text{ nm}$, $\epsilon = 11900$

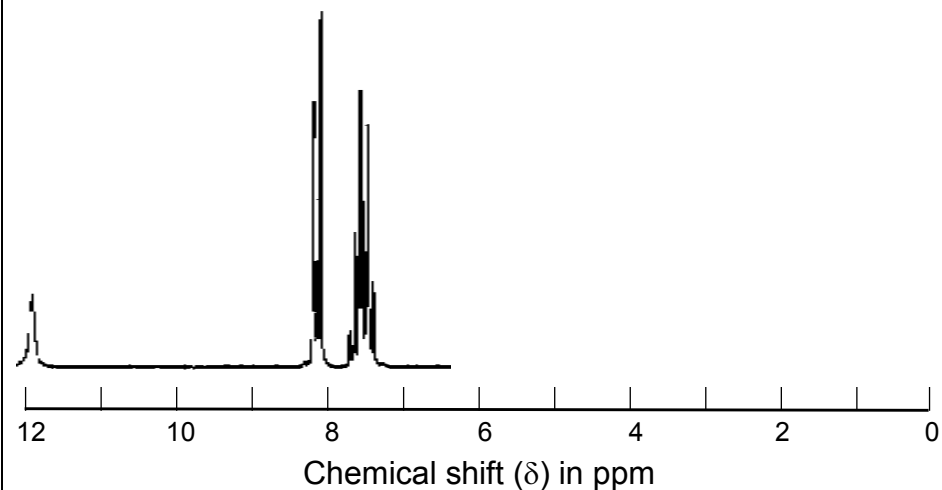
Analysis

Carbon	68.9%	Oxygen	26.2%
Hydrogen	4.9%		

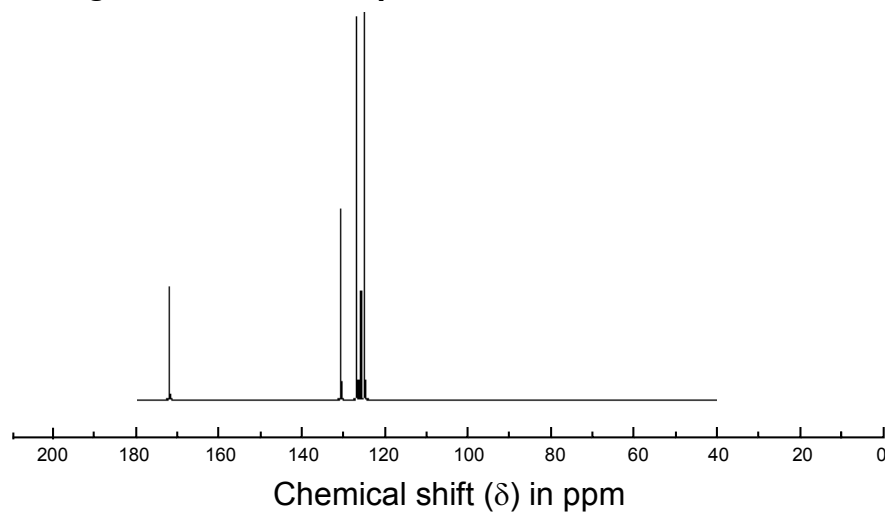
Infra-red spectrum



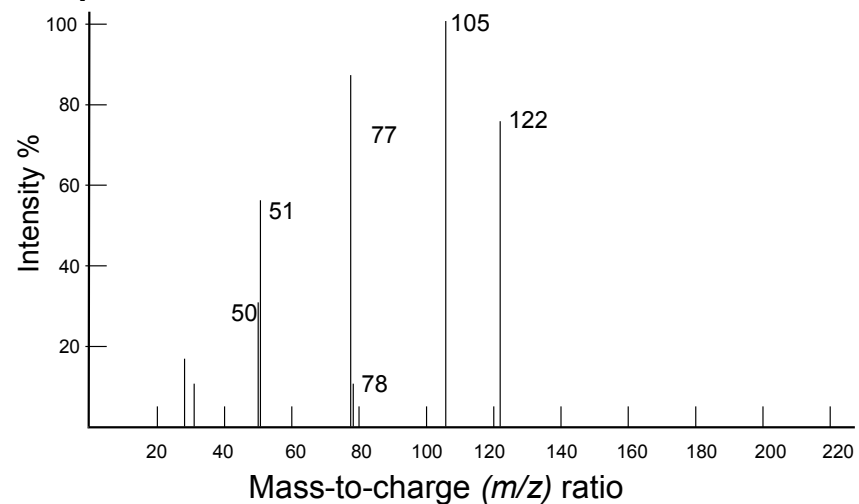
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 3

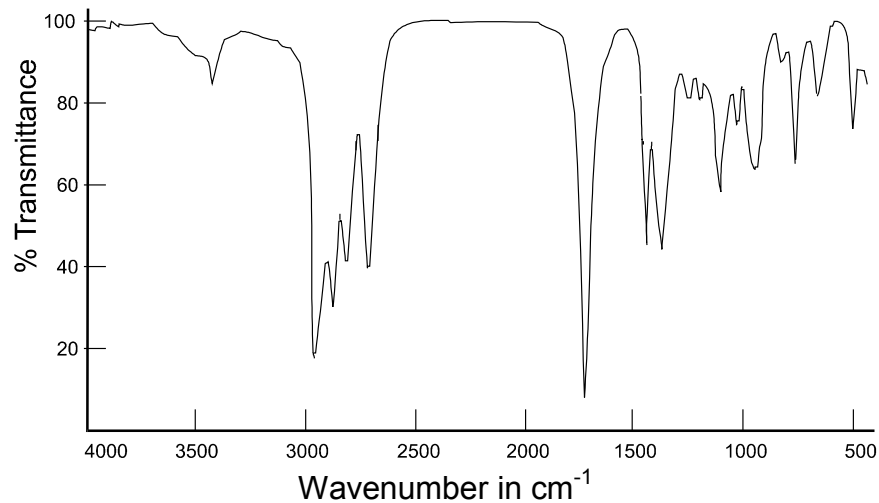
Ultra-violet spectrum

$\lambda = 225 \text{ nm}$, $\epsilon = 13$

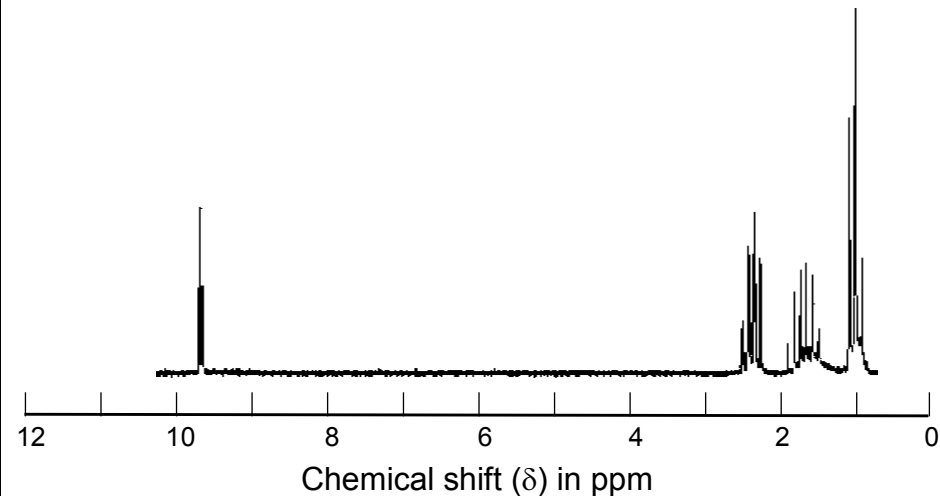
Analysis

Carbon	66.7%	Oxygen	22.2%
Hydrogen	11.1%		

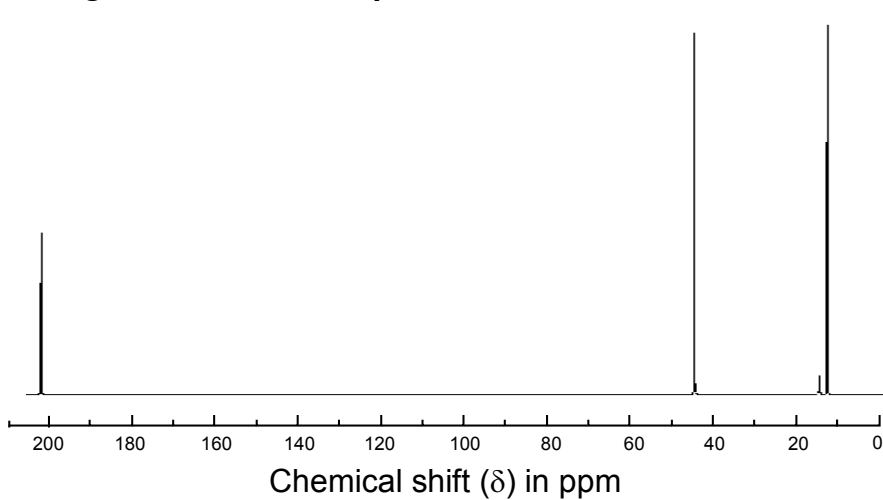
Infra-red spectrum



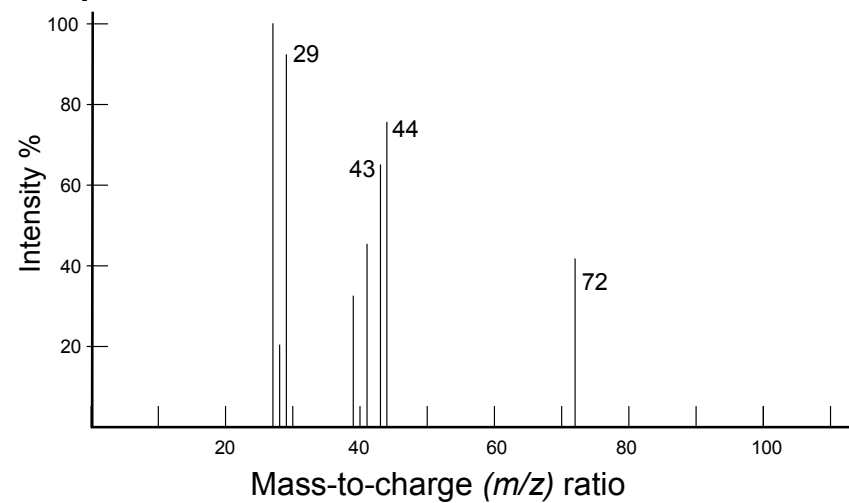
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 4

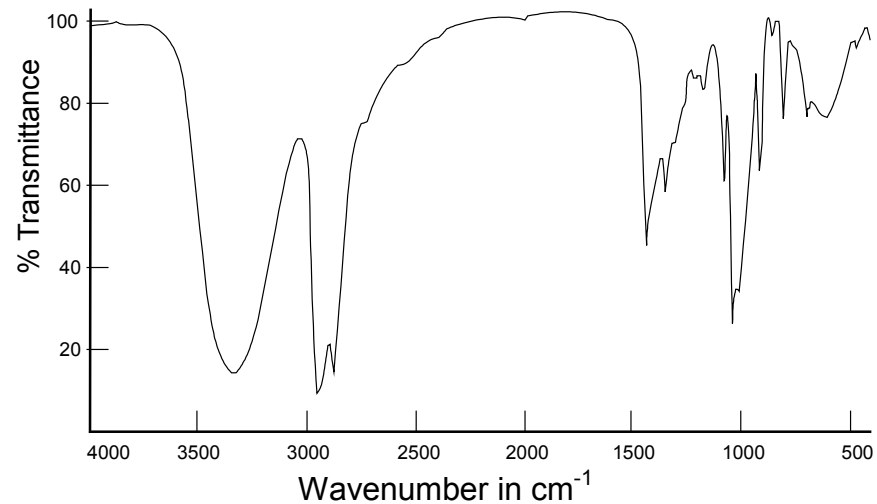
Ultra-violet spectrum

$\lambda = 280 \text{ nm}$, $\epsilon = 686$

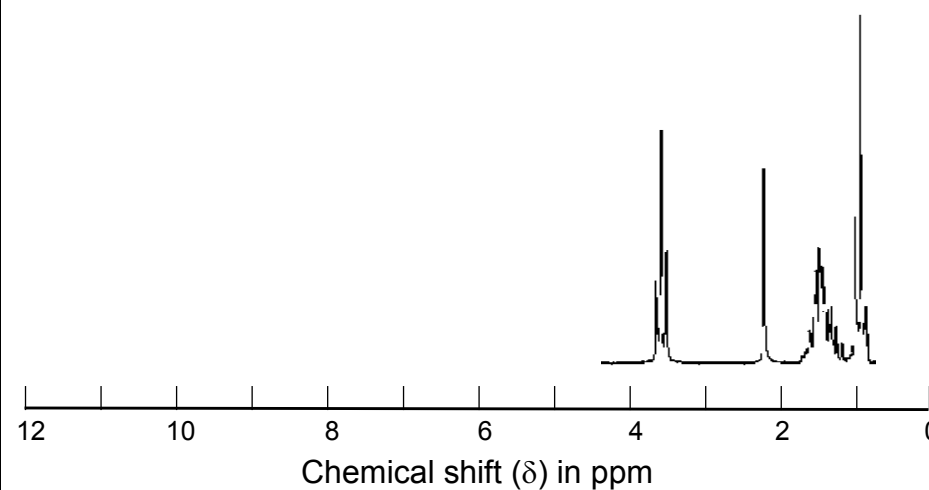
Analysis

Carbon	64.9%	Oxygen	21.6%
Hydrogen	13.5%		

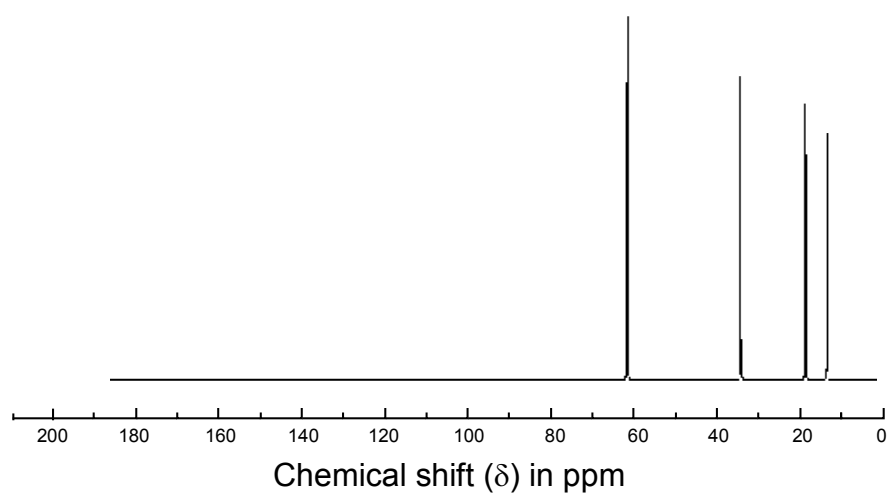
Infra-red spectrum



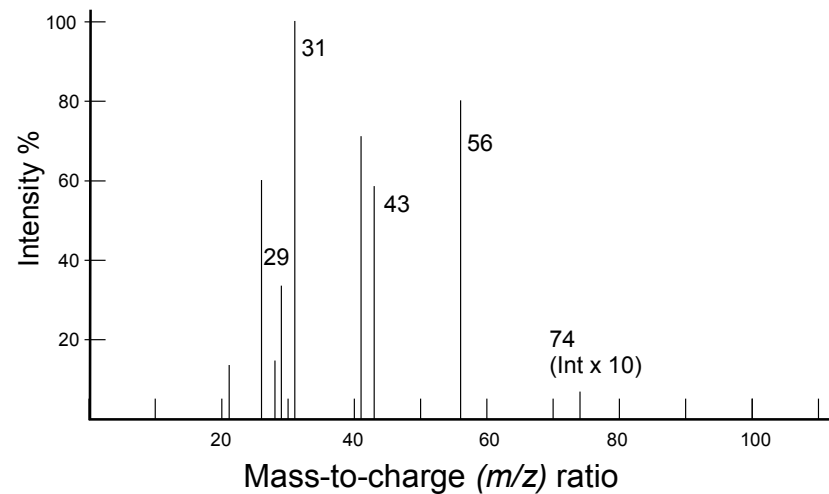
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 5

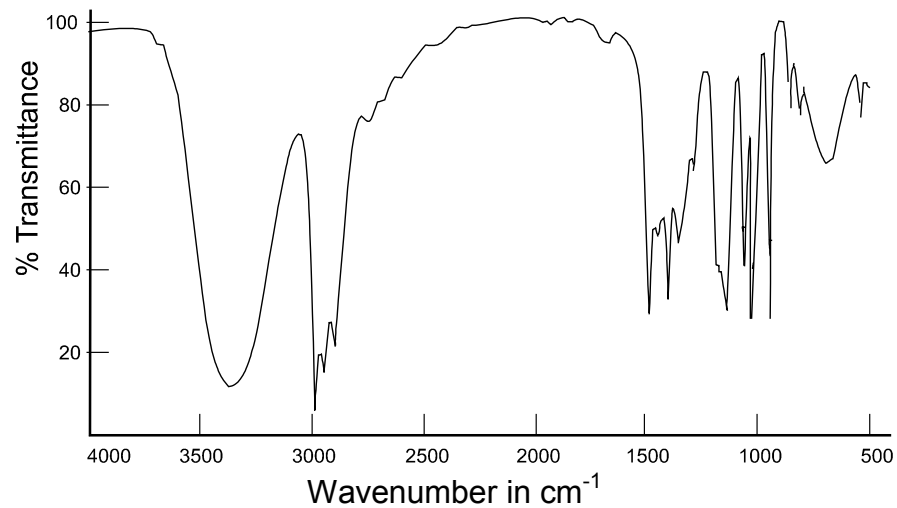
Ultra-violet spectrum

$\lambda = 211 \text{ nm}$, $\epsilon = 32$

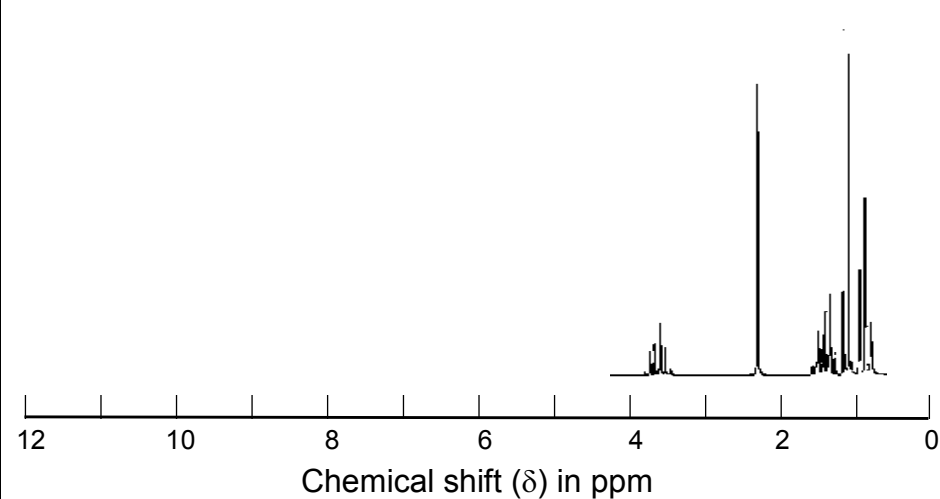
Analysis

Carbon	64.9%	Oxygen	21.6%
Hydrogen	13.5%		

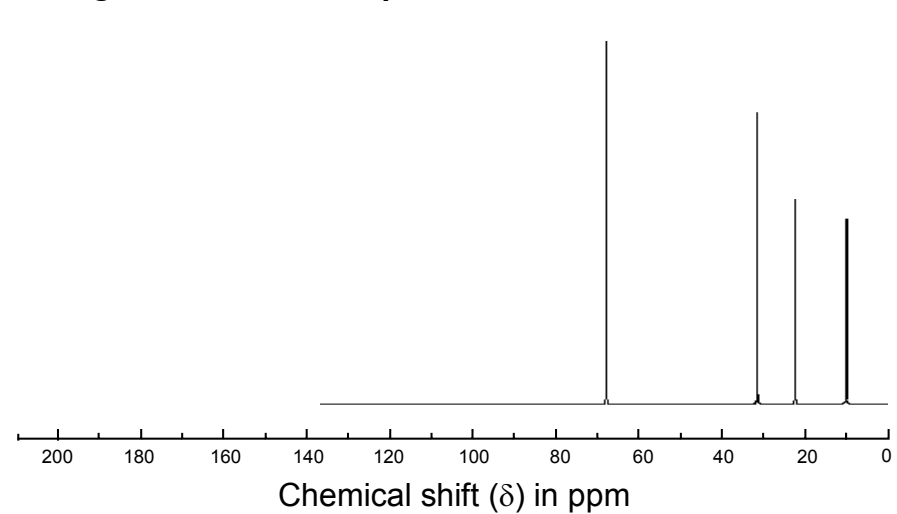
Infra-red spectrum



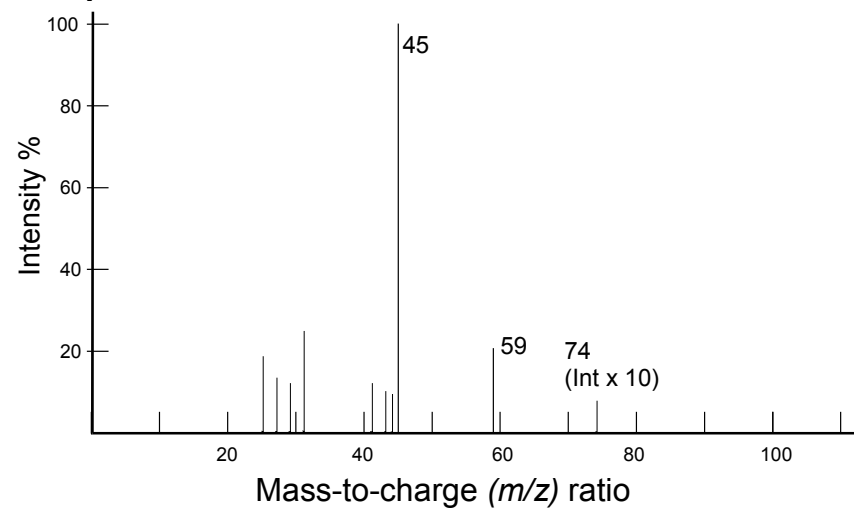
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 6

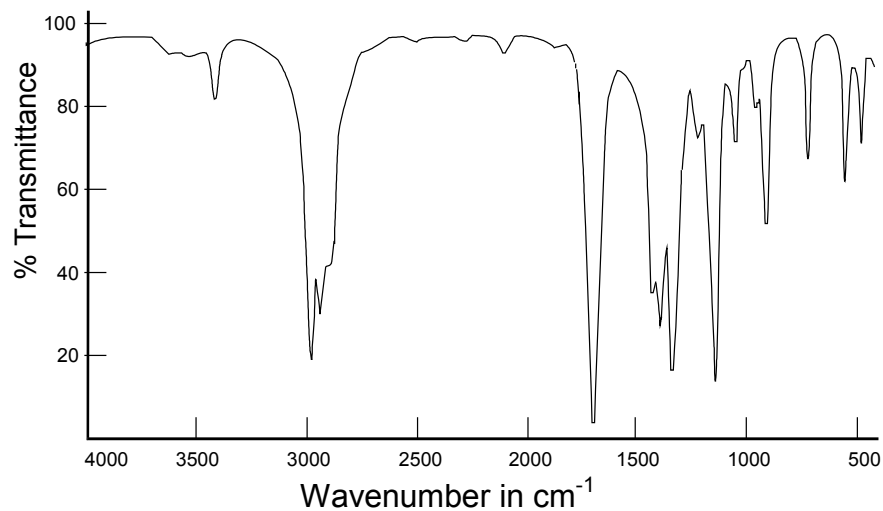
Ultra-violet spectrum

$\lambda = 279 \text{ nm}$, $\epsilon = 16$

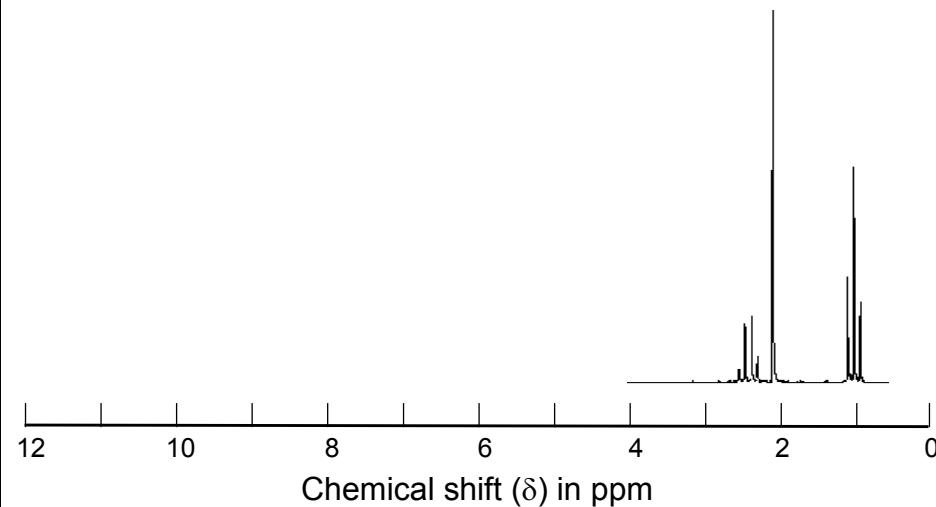
Analysis

Carbon	66.7%	Oxygen	22.2%
Hydrogen	11.1%		

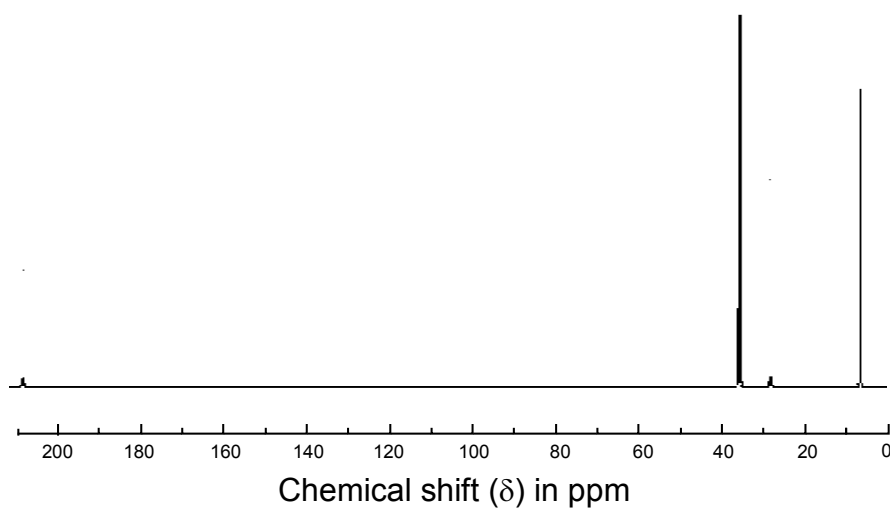
Infra-red spectrum



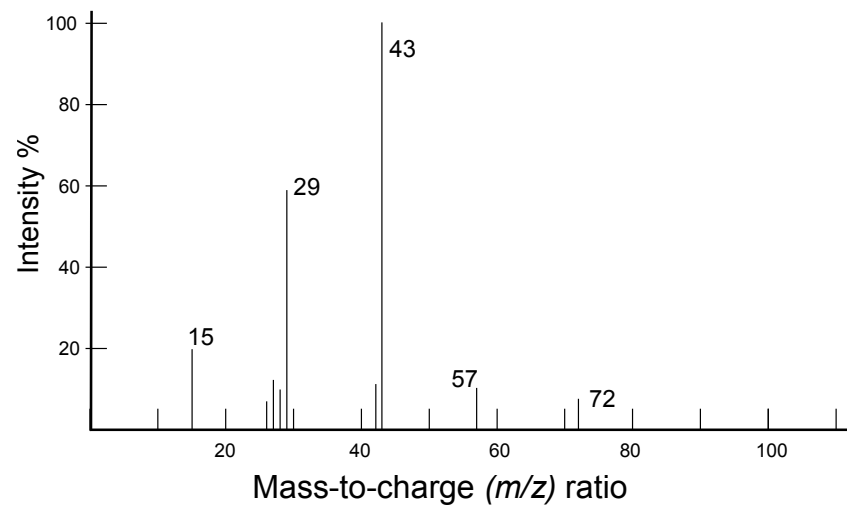
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 7

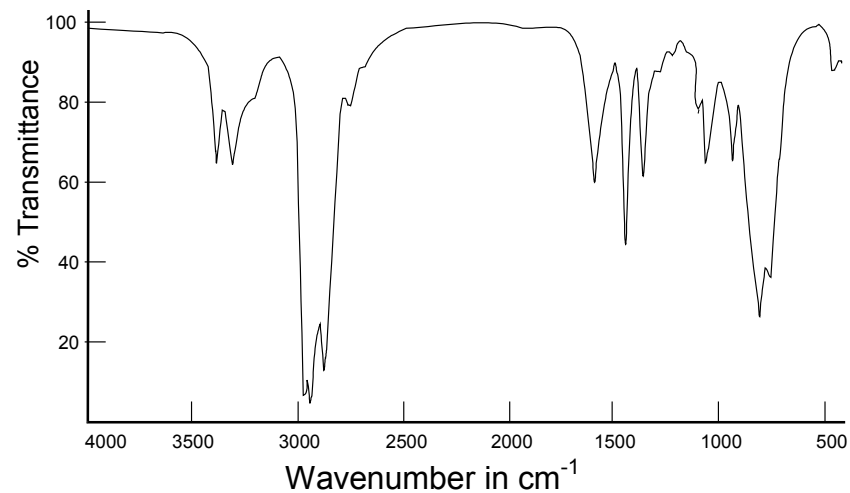
Ultra-violet spectrum

No data available

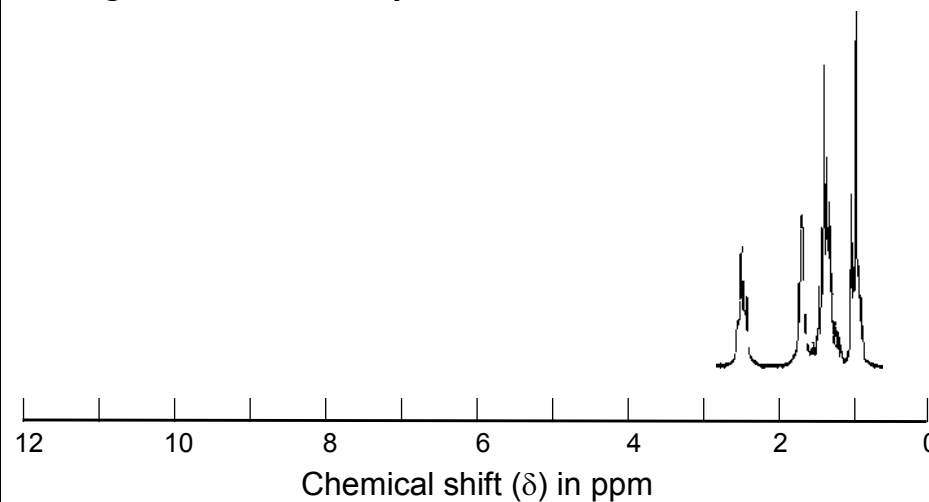
Analysis

Carbon	65.8%	Nitrogen	19.2%
Hydrogen	15.1%		

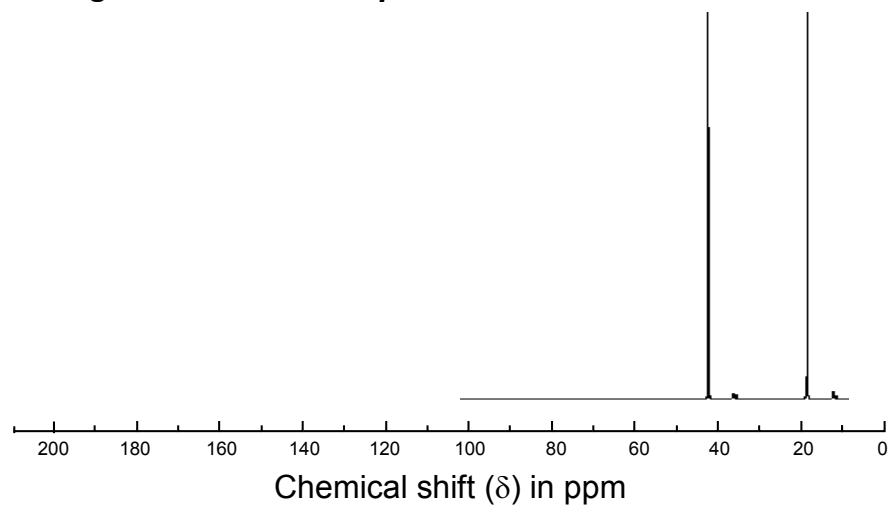
Infra-red spectrum



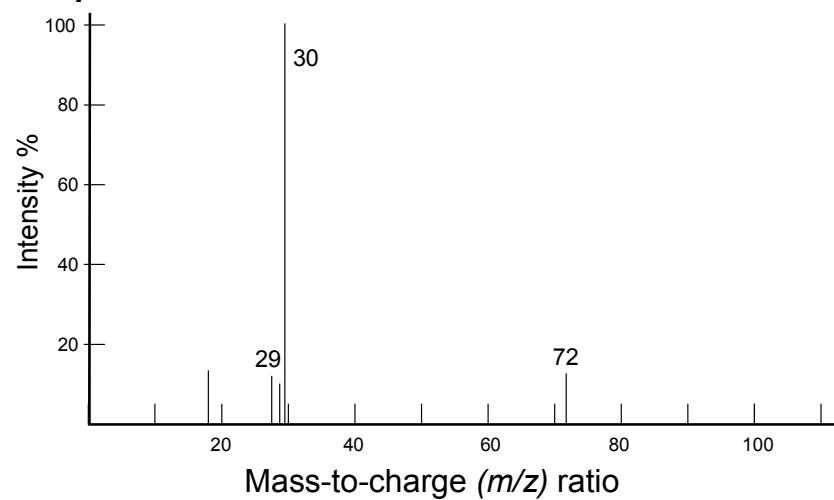
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum

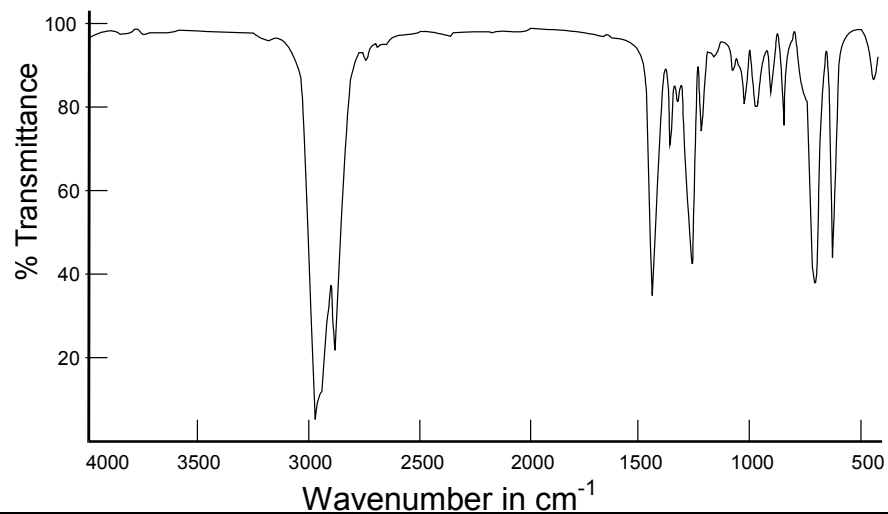
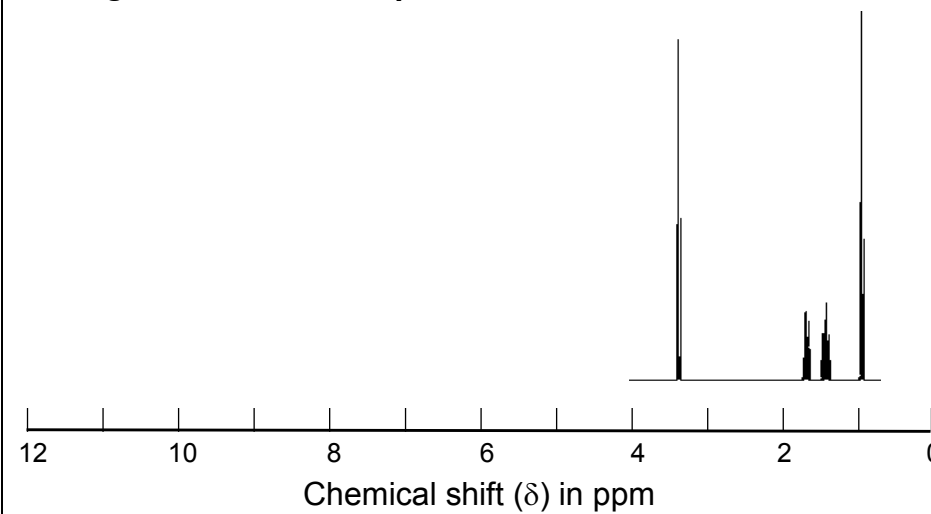
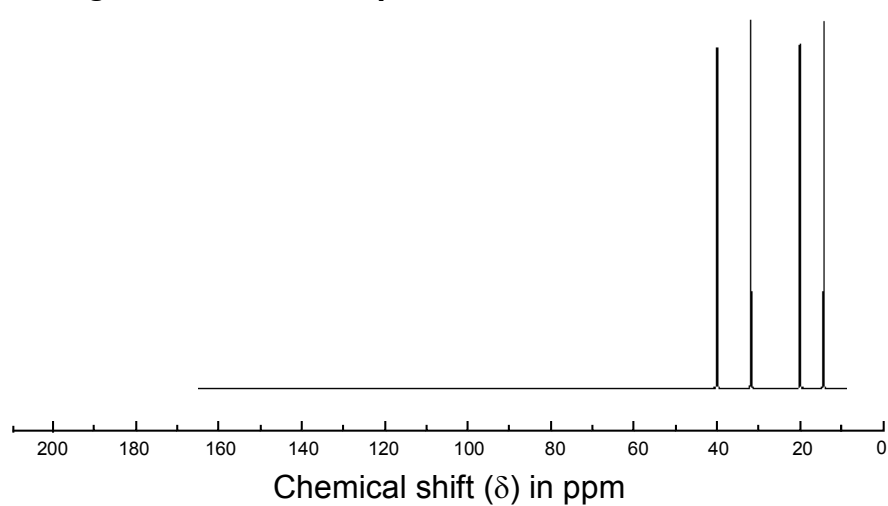
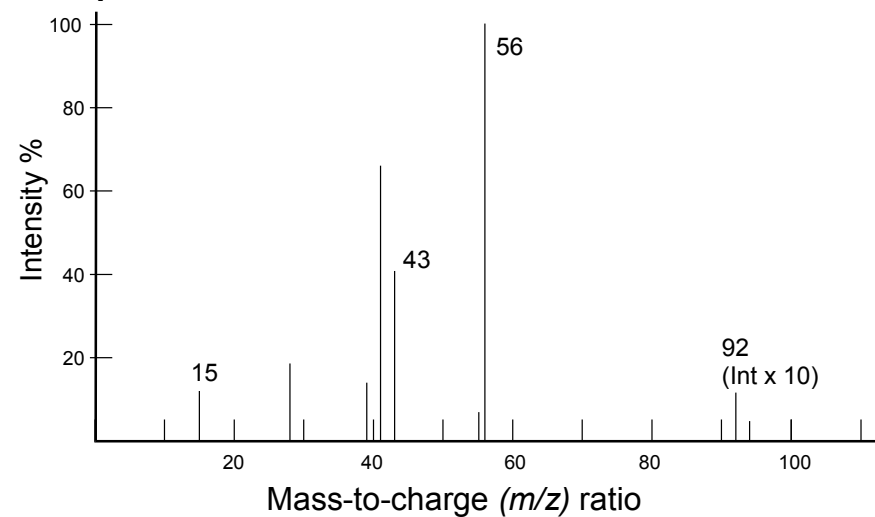


Substance 8**Ultra-violet spectrum**

No data available

Analysis

Carbon	51.9%	Chlorine	38.4%
Hydrogen	9.7%		

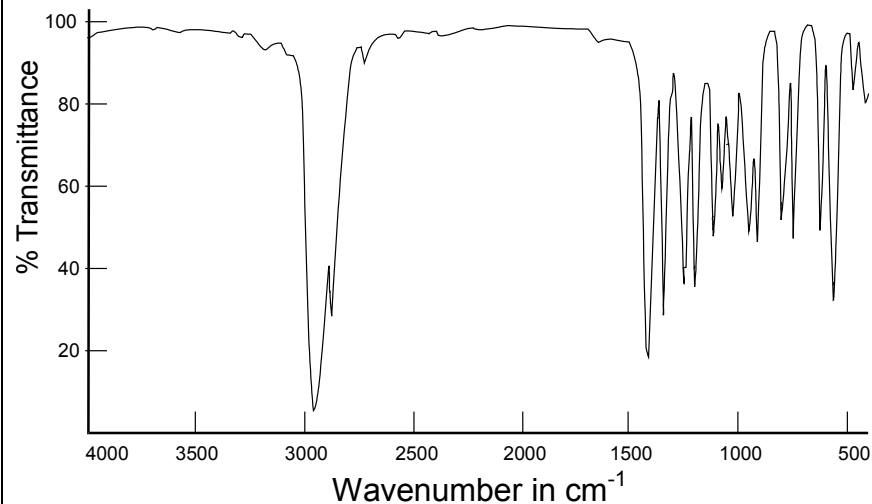
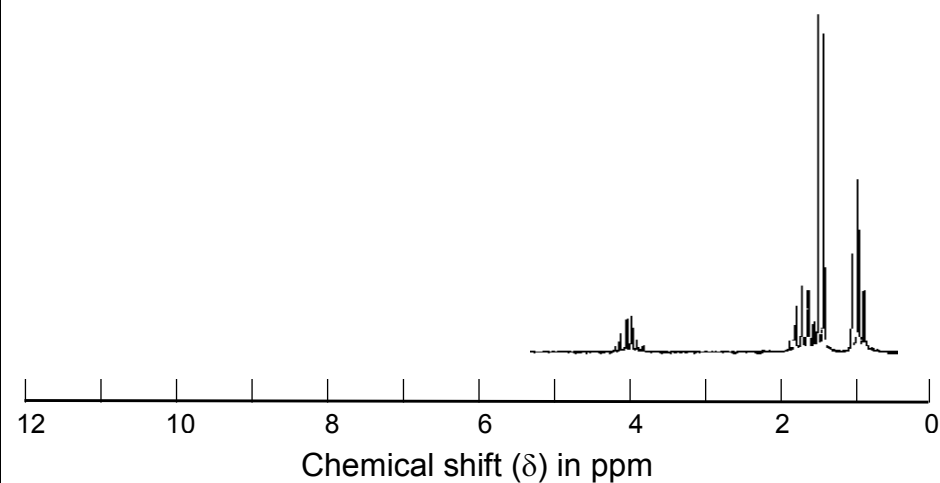
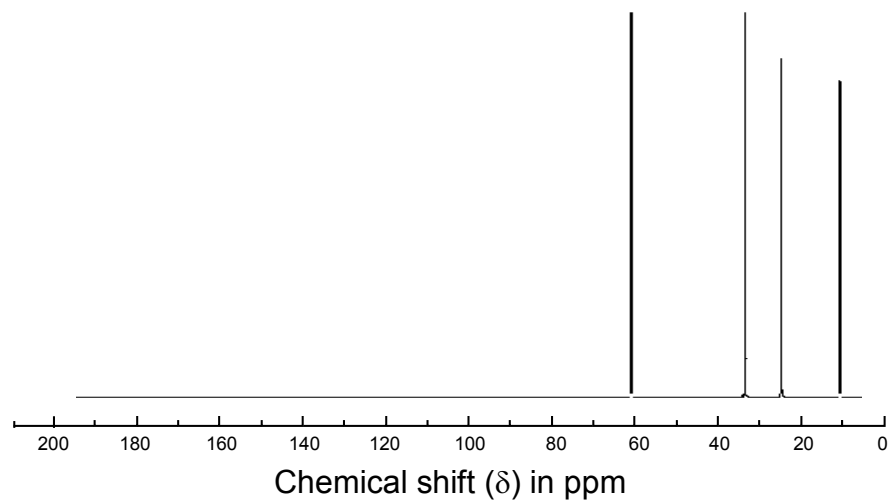
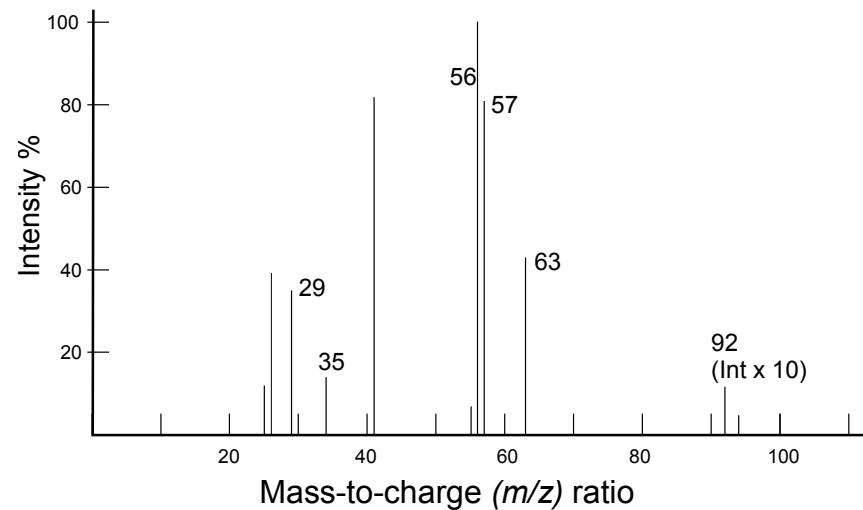
Infra-red spectrum**¹H magnetic resonance spectrum****¹³C magnetic resonance spectrum****Mass spectrum**

Substance 9**Ultra-violet spectrum**

No data available

Analysis

Carbon	51.9%	Chlorine	38.4%
Hydrogen	9.7%		

Infra-red spectrum**¹H magnetic resonance spectrum****¹³C magnetic resonance spectrum****Mass spectrum**

Substance 10

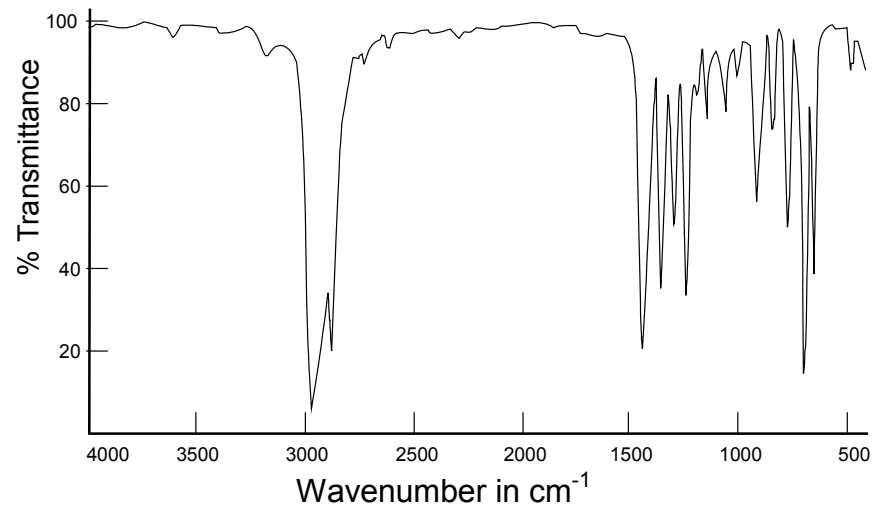
Ultra-violet spectrum

No data available

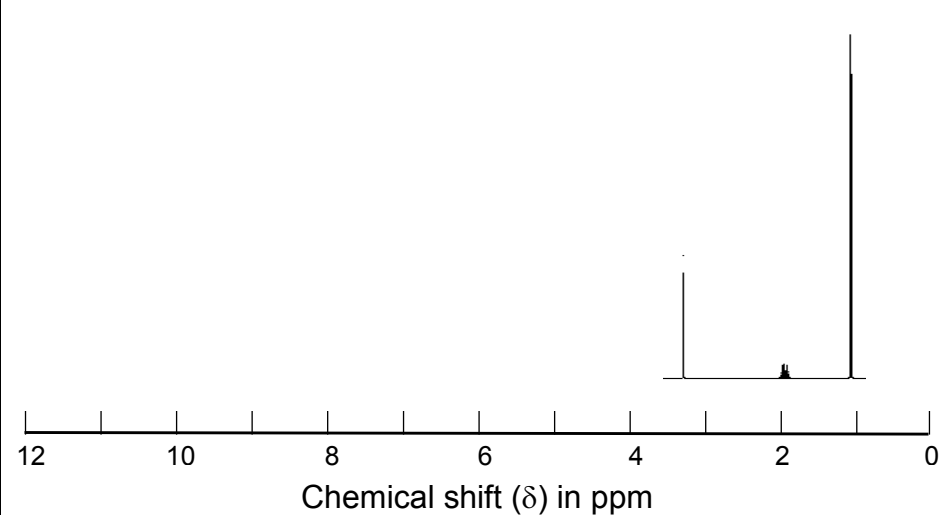
Analysis

Carbon	51.9%	Chlorine	38.4%
Hydrogen	9.7%		

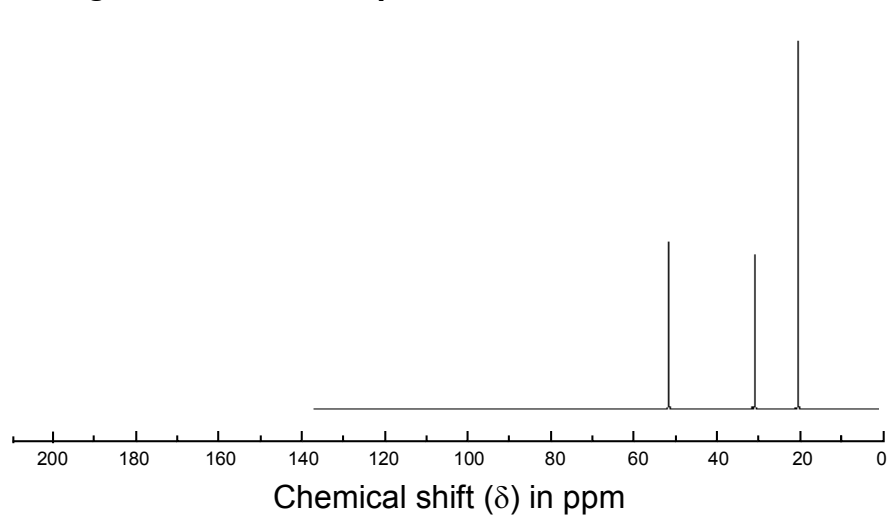
Infra-red spectrum



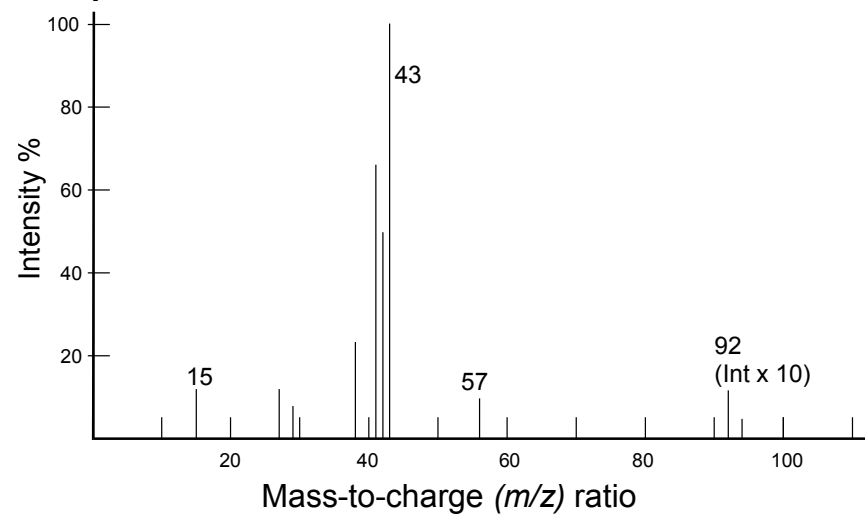
¹H magnetic resonance spectrum



¹³C magnetic resonance spectrum



Mass spectrum

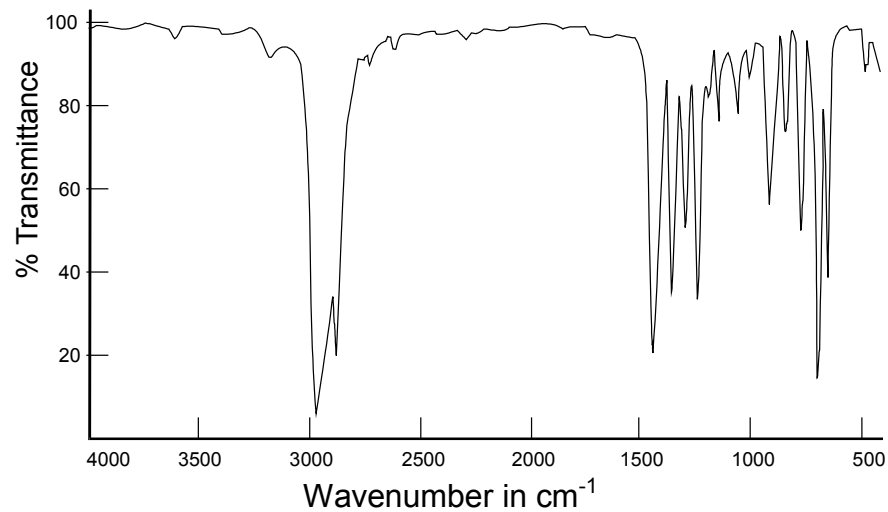
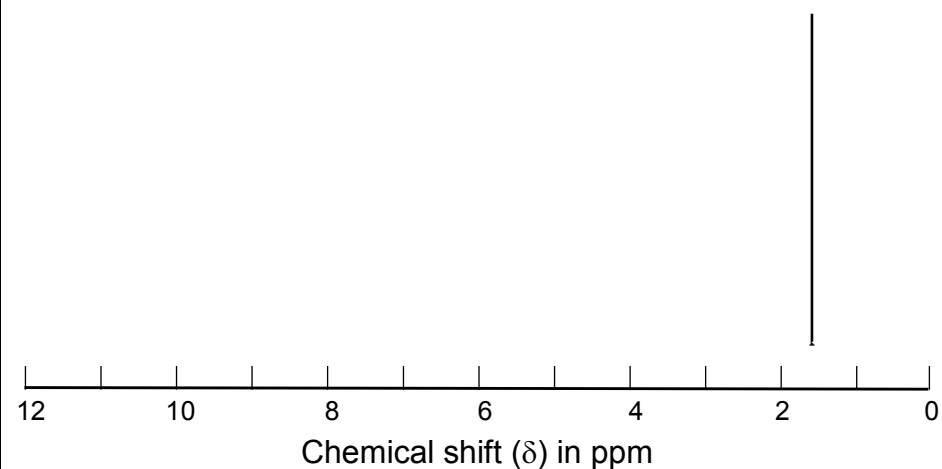
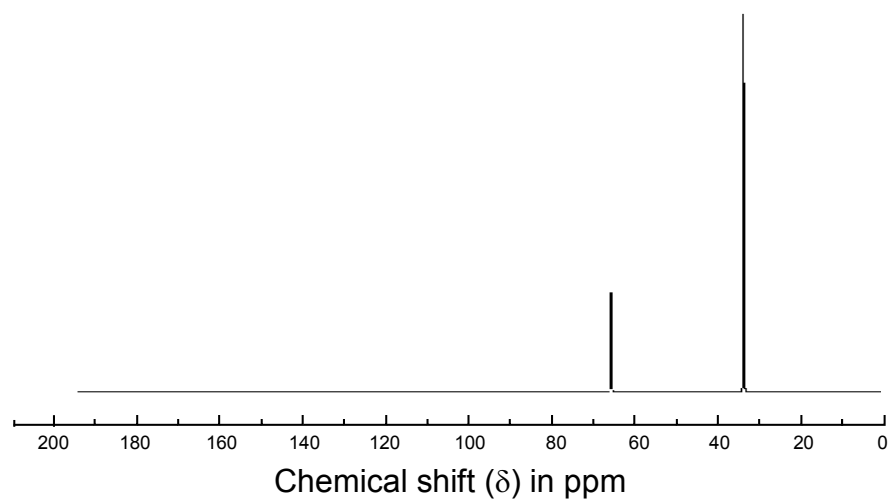
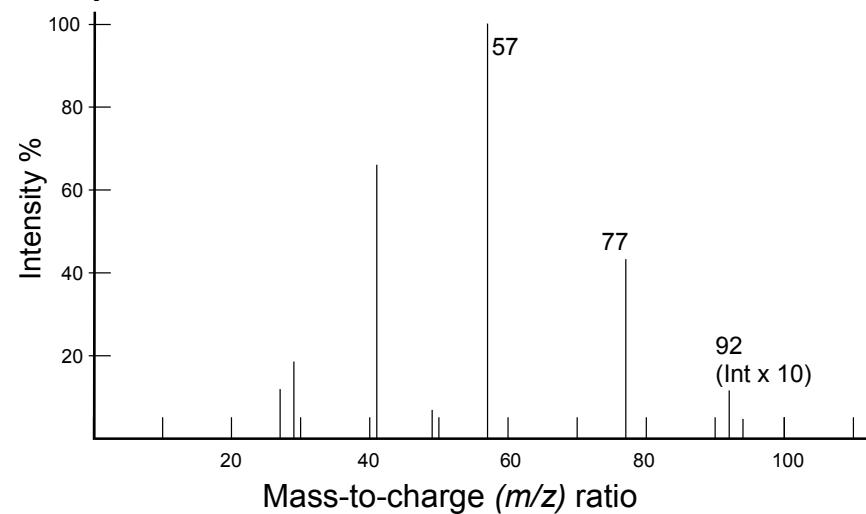


Substance 11**Ultra-violet spectrum**

No data available

Analysis

Carbon	51.9%	Chlorine	38.4%
Hydrogen	9.7%		

Infra-red spectrum**¹H magnetic resonance spectrum****¹³C magnetic resonance spectrum****Mass spectrum**

Substance 12

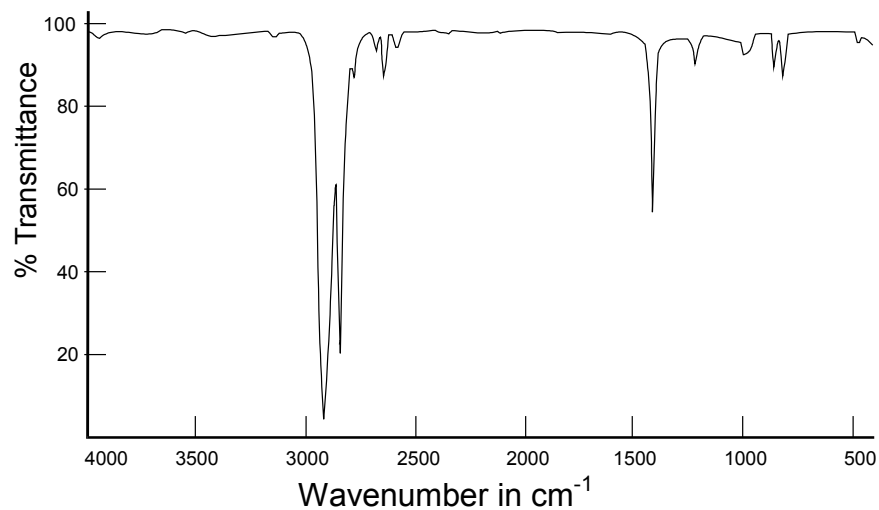
Ultra-violet spectrum

No data available

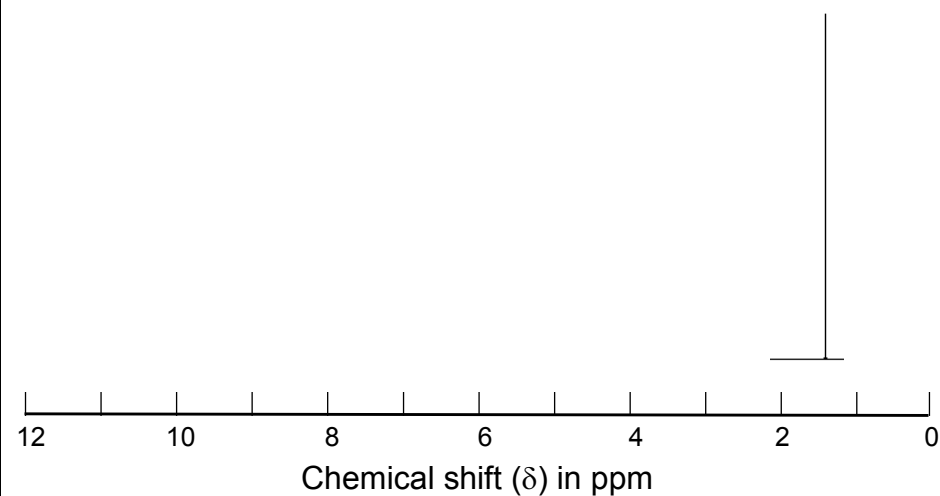
Analysis

Carbon 85.7%
Hydrogen 14.3%

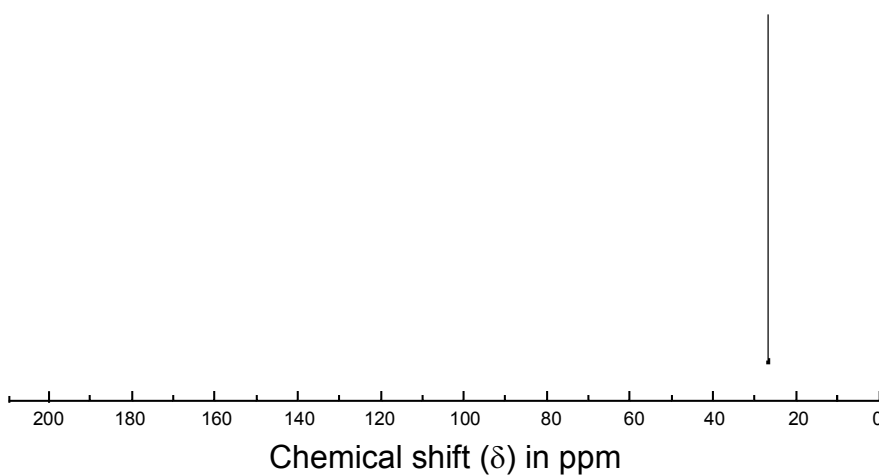
Infra-red spectrum



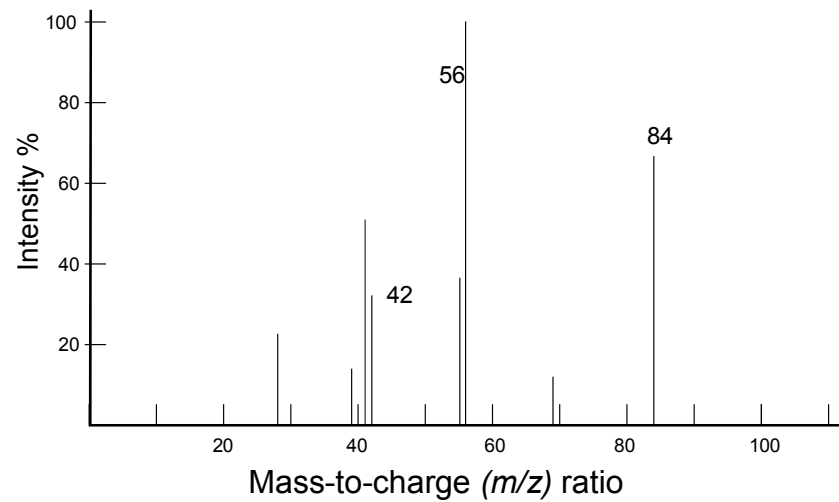
¹H magnetic resonance spectrum



¹³C magnetic resonance spectrum



Mass spectrum



Substance 13

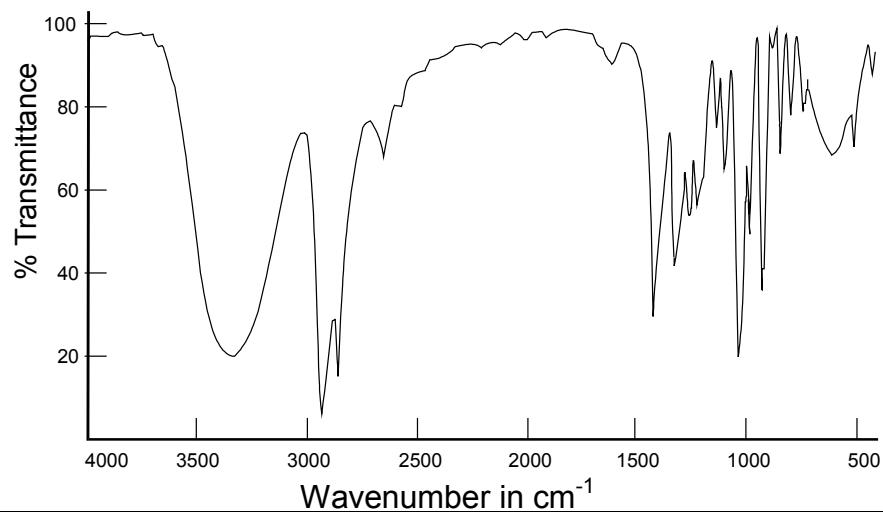
Ultra-violet spectrum

No data available

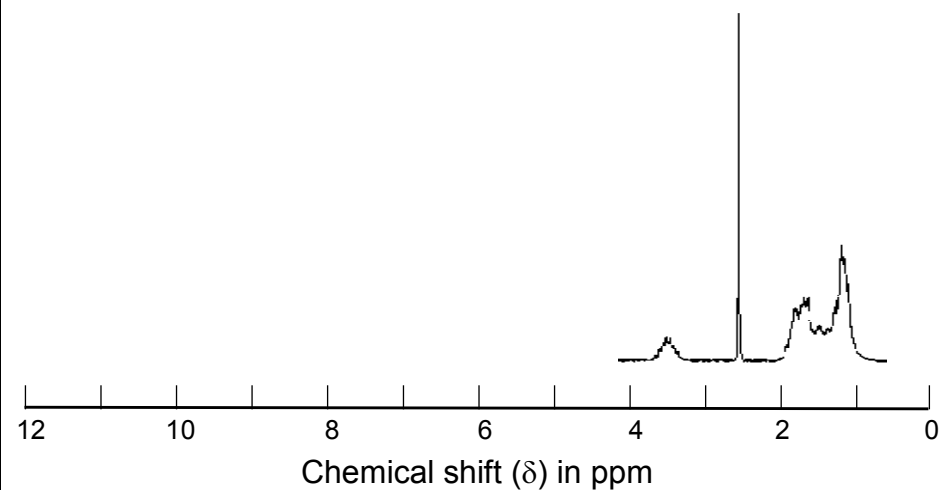
Analysis

Carbon	72.0%	Oxygen	16.0%
Hydrogen	12.0%		

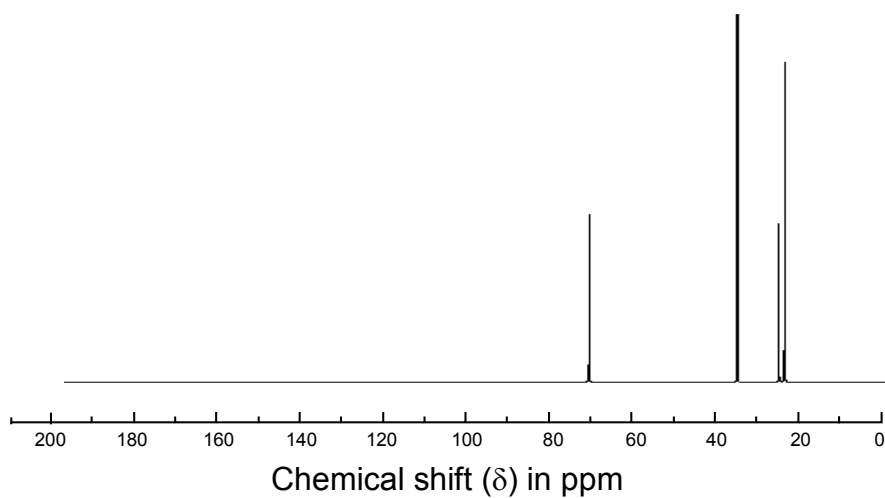
Infra-red spectrum



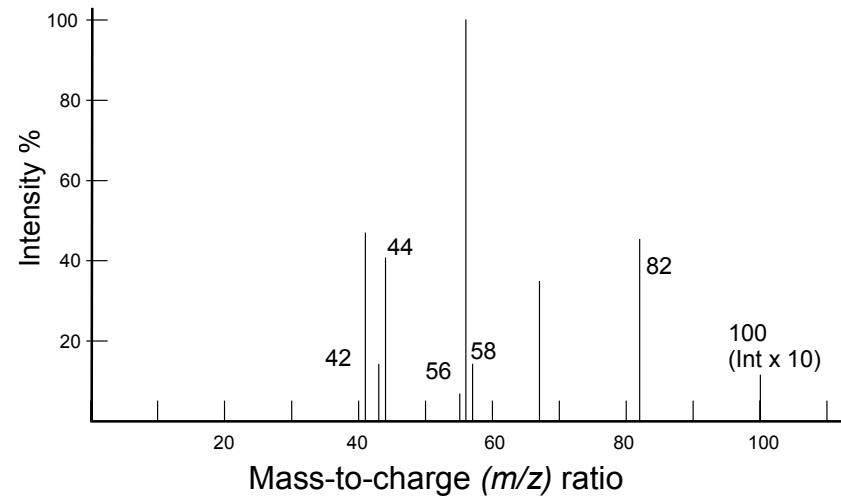
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 14

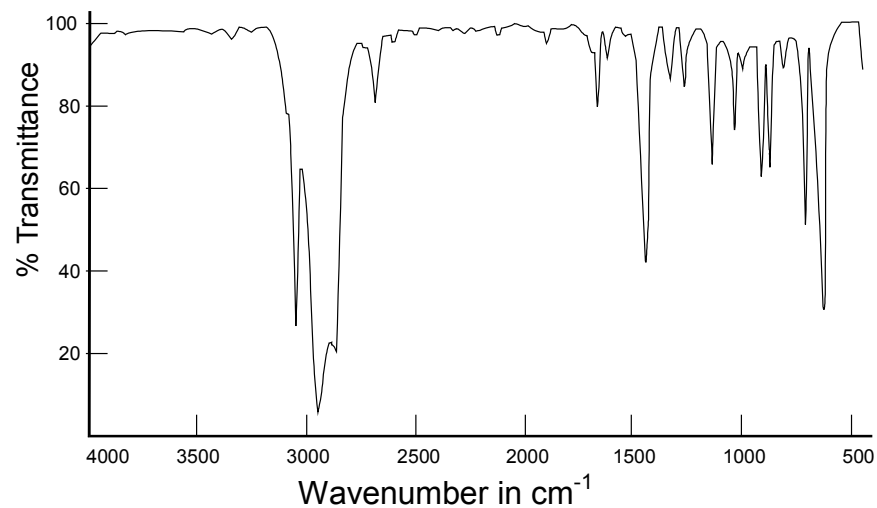
Ultra-violet spectrum

No data available

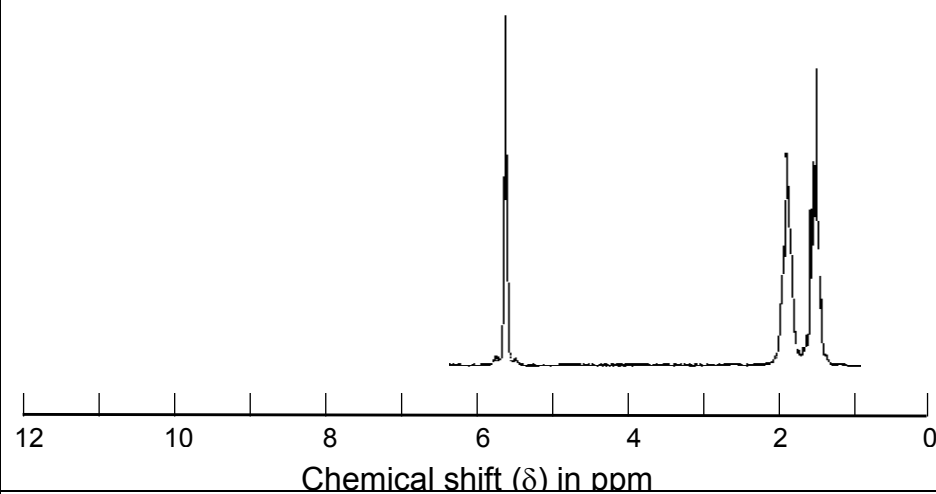
Analysis

Carbon 87.8%
Hydrogen 12.2%

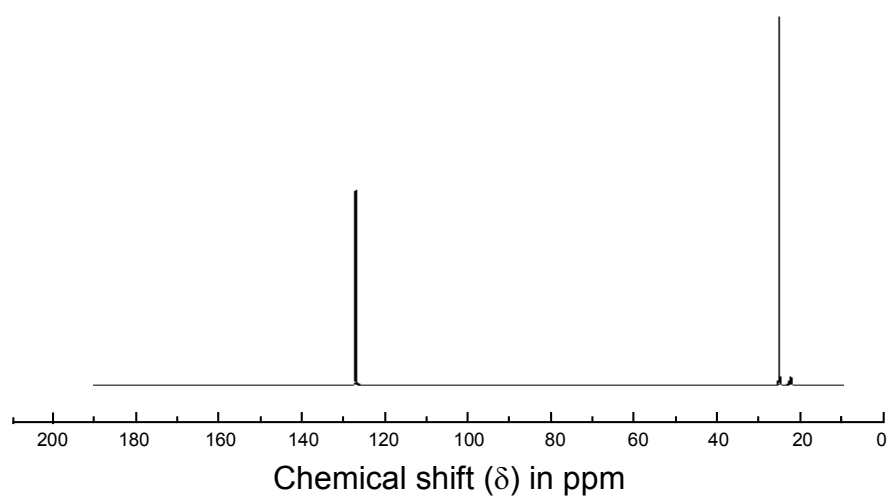
Infra-red spectrum



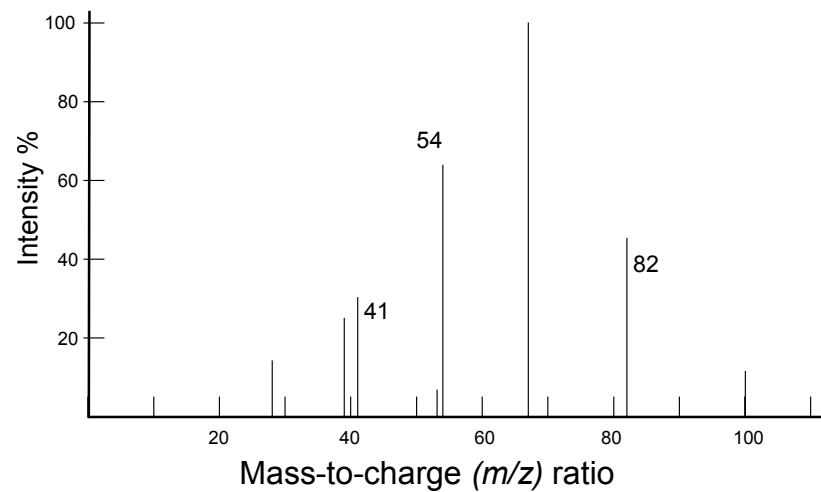
¹H magnetic resonance spectrum



¹³C magnetic resonance spectrum



Mass spectrum



Substance 15

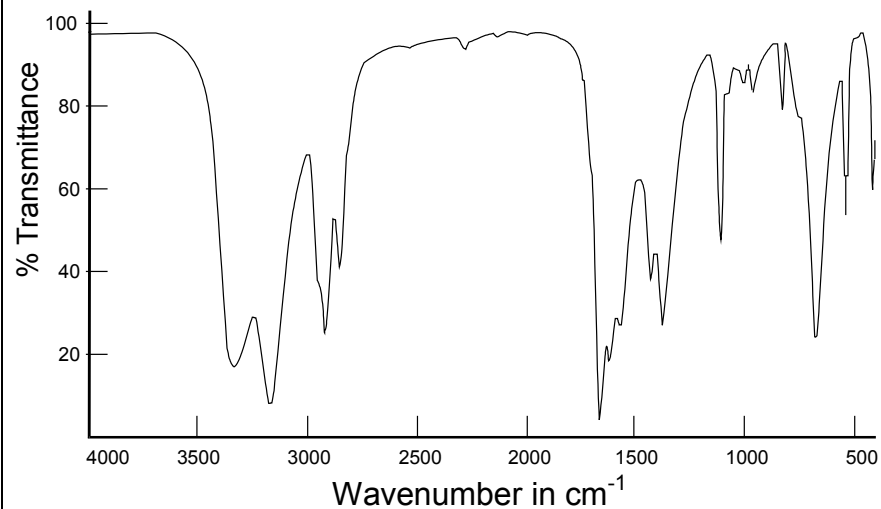
Ultra-violet spectrum

$\lambda = 185 \text{ nm}$, $\epsilon = 8710$

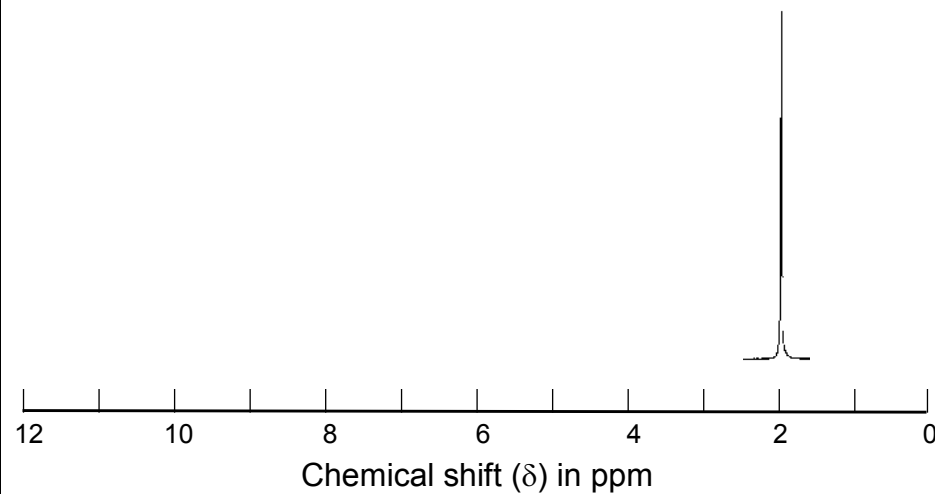
Analysis

Carbon	40.7%	Oxygen	27.1%
Hydrogen	8.5%	Nitrogen	23.7%

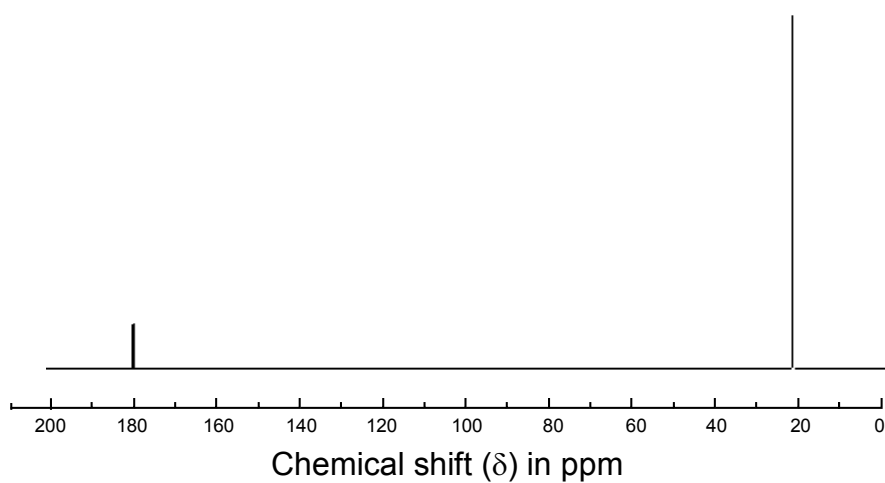
Infra-red spectrum



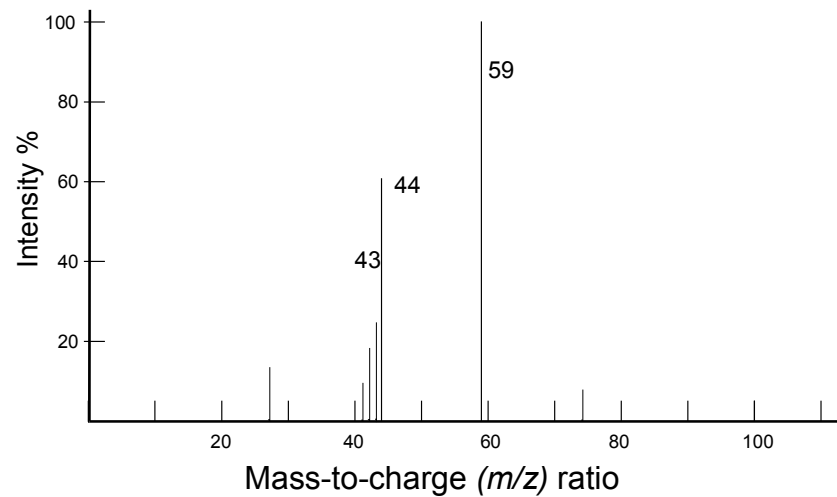
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 16

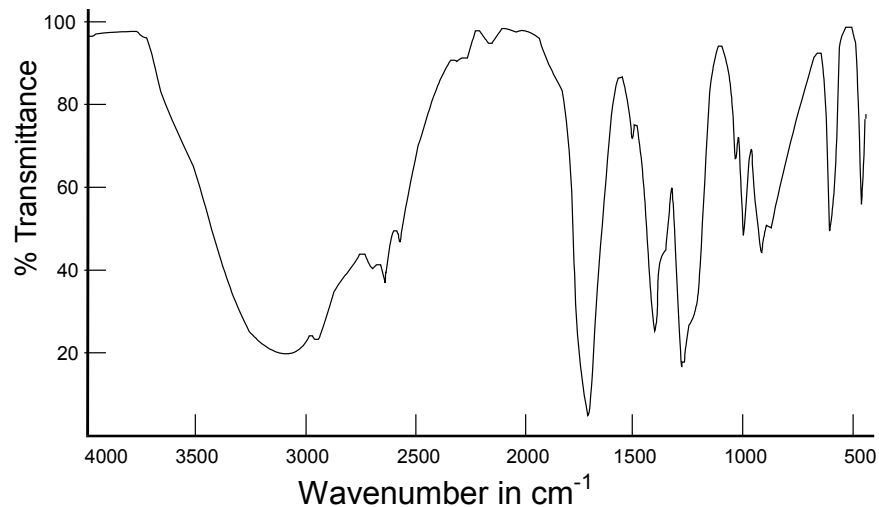
Ultra-violet spectrum

$\lambda = 208 \text{ nm}$, $\epsilon = 32$

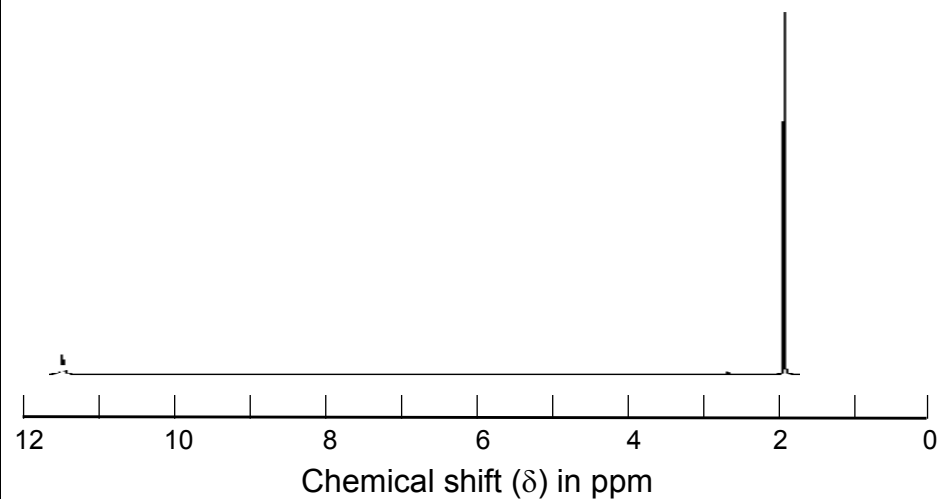
Analysis

Carbon	40.0%	Oxygen	53.3%
Hydrogen	6.7%		

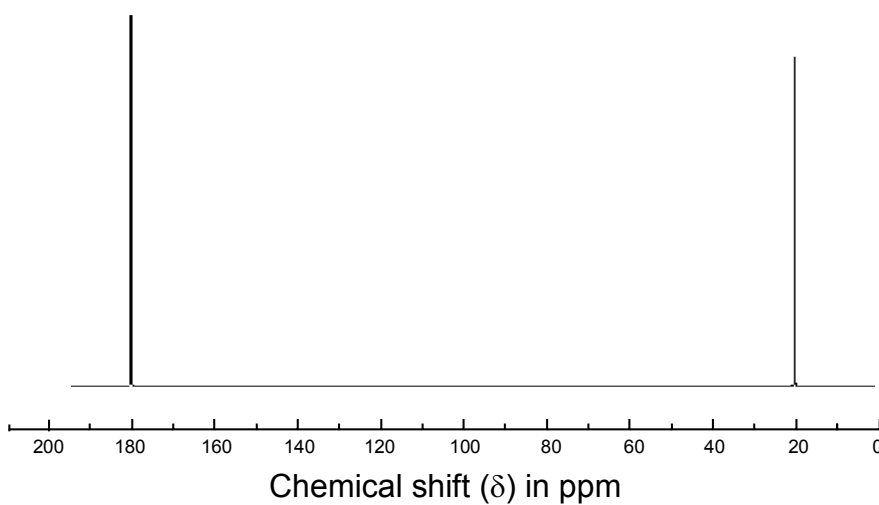
Infra-red spectrum



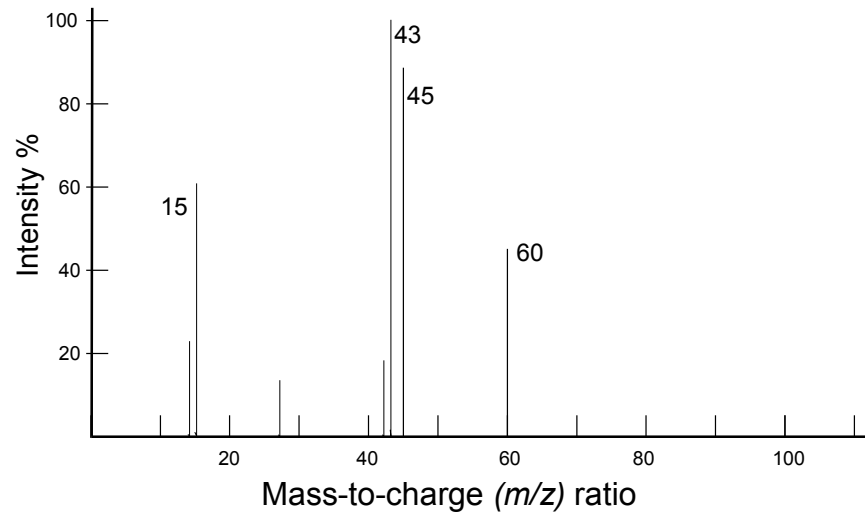
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 17

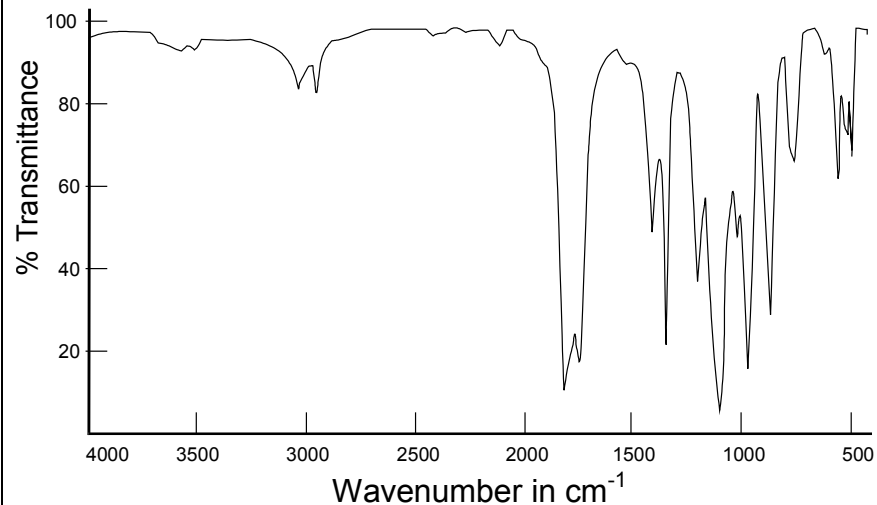
Ultra-violet spectrum

$\lambda = 225 \text{ nm}$, $\epsilon = 48$

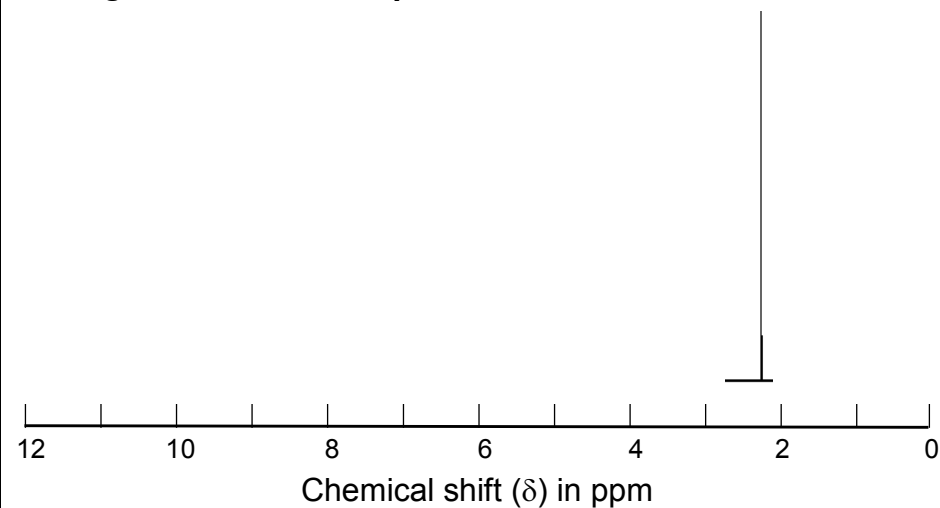
Analysis

Carbon	47.1%	Oxygen	47.1%
Hydrogen	5.9%		

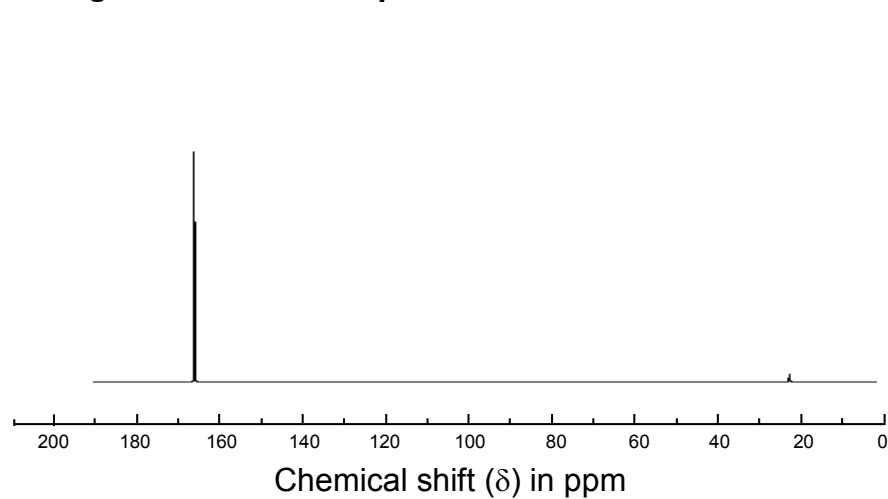
Infra-red spectrum



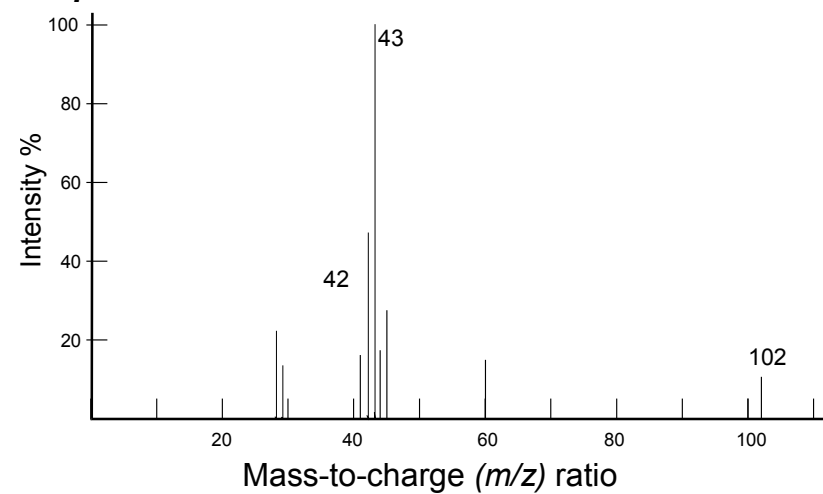
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 18

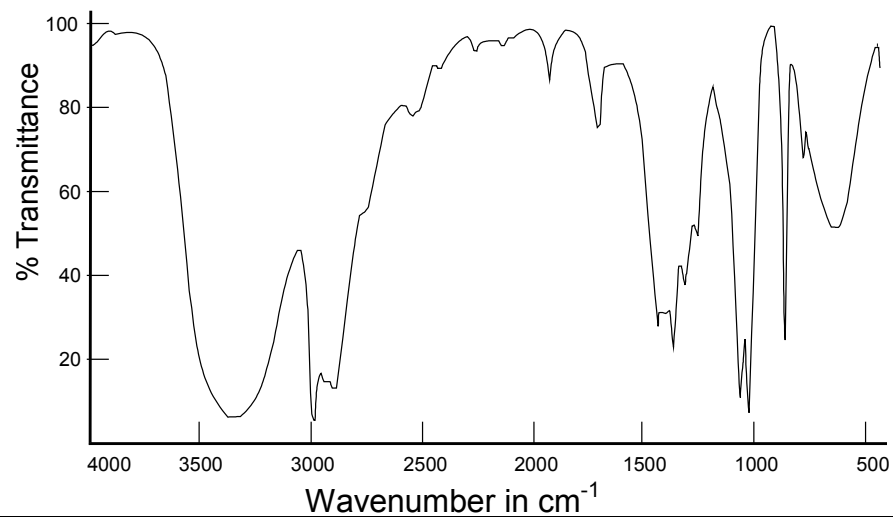
Ultra-violet spectrum

No data available

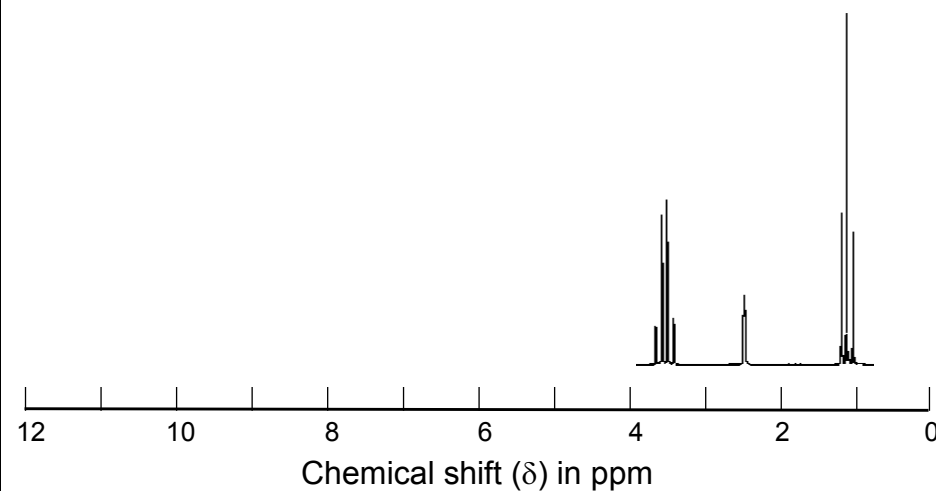
Analysis

Carbon	52.1%	Oxygen	34.8%
Hydrogen	13.0%		

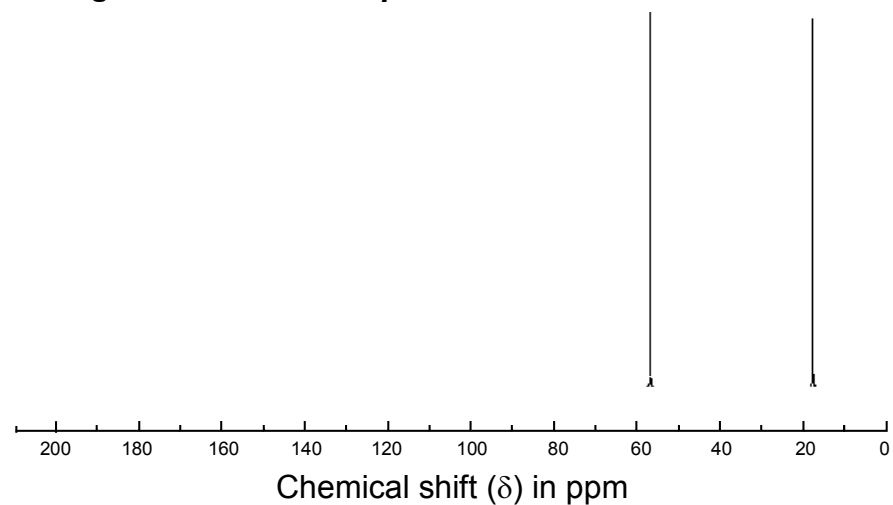
Infra-red spectrum



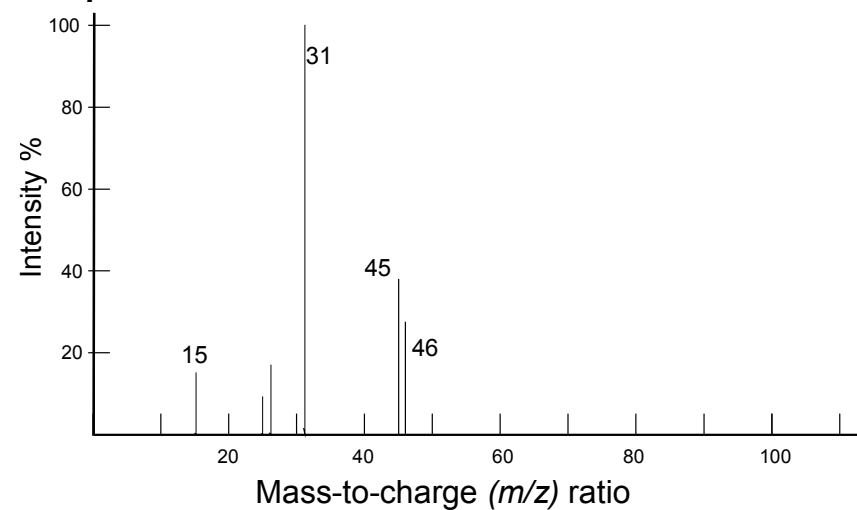
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 19

Ultra-violet spectrum

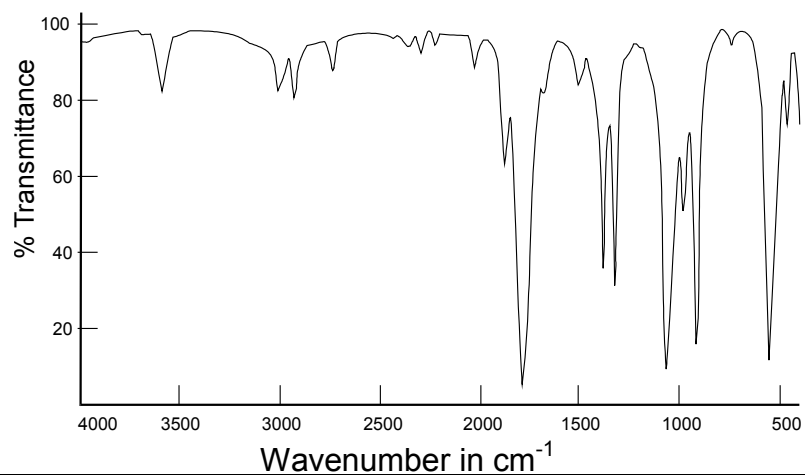
$\lambda = 242 \text{ nm}$, $\epsilon = 41$

$\lambda = 198 \text{ nm}$, $\epsilon = 24$

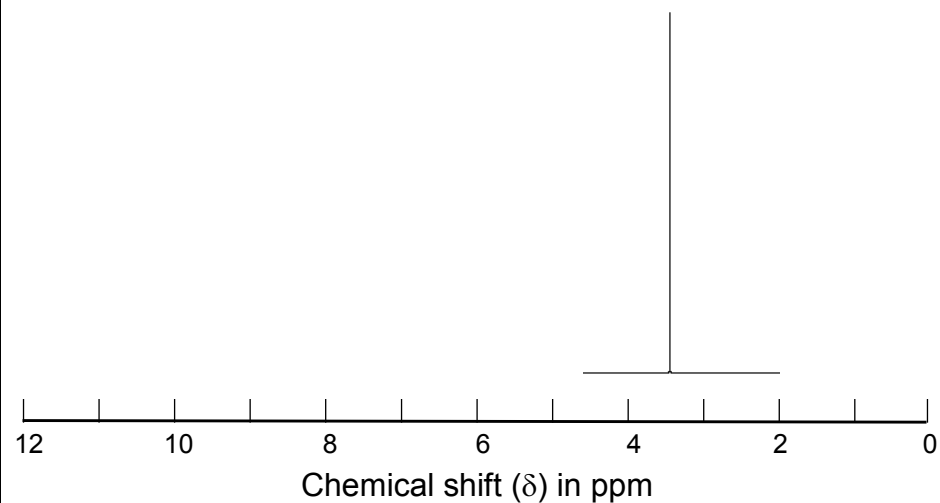
Analysis

Carbon	30.6%	Oxygen	20.4%
Hydrogen	3.8%	Chlorine	45.2%

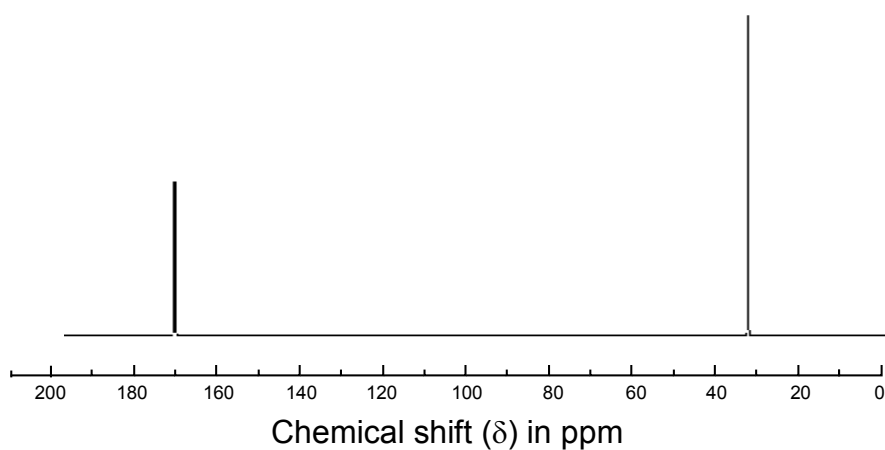
Infra-red spectrum



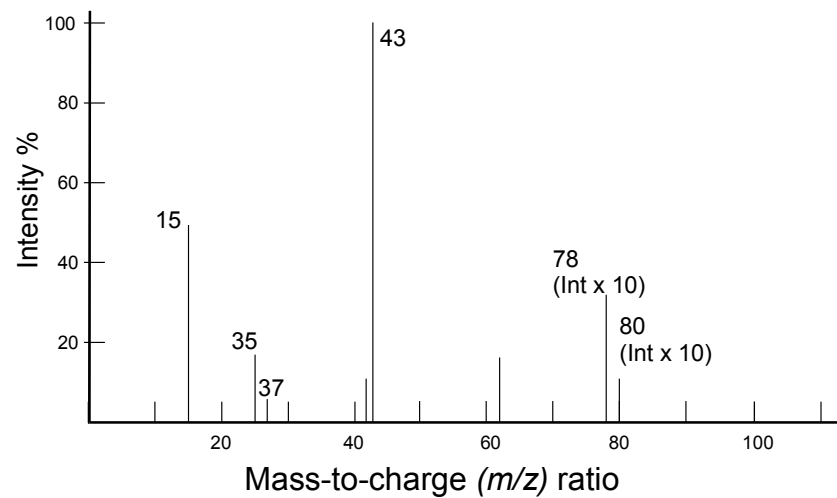
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 20

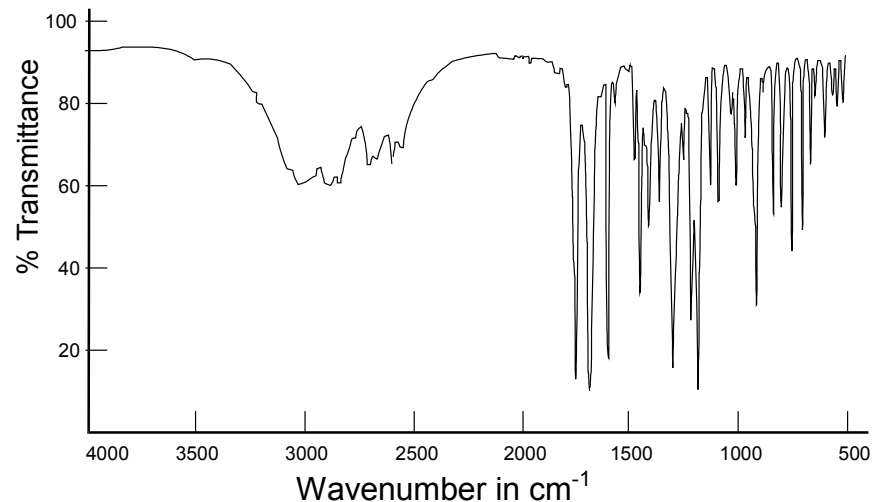
Ultra-violet spectrum

$\lambda = 225 \text{ nm}$, $\epsilon = 48$

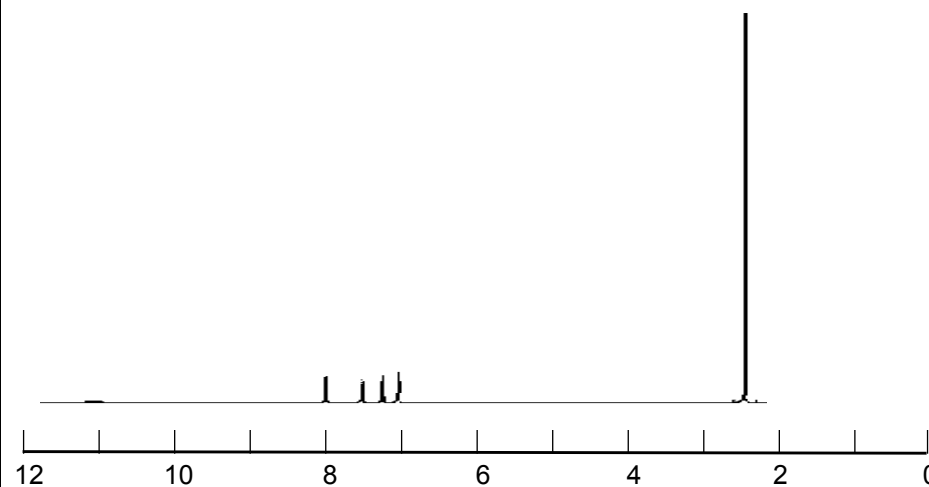
Analysis

Carbon	60.0%	Oxygen	35.6%
Hydrogen	4.4%		

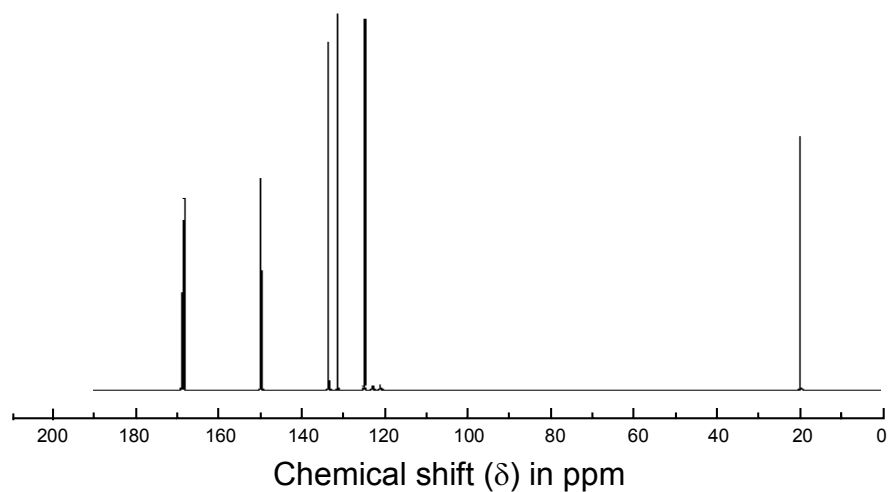
Infra-red spectrum



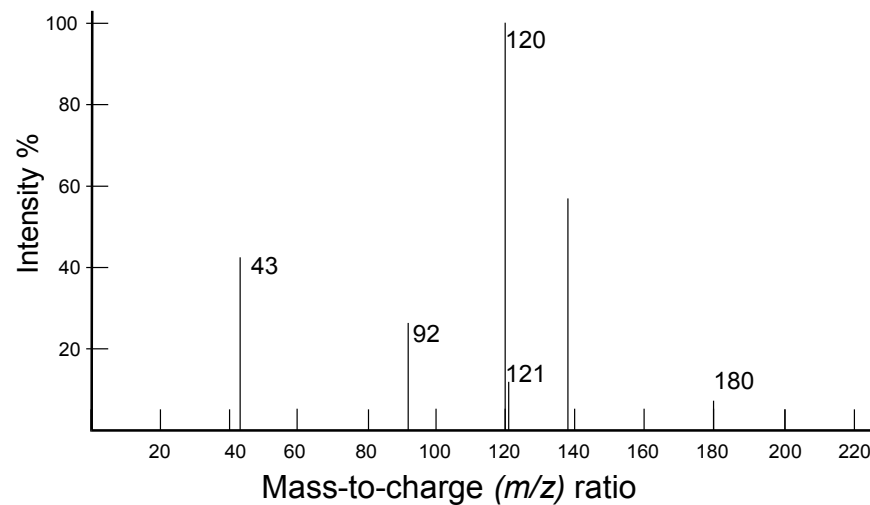
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 21

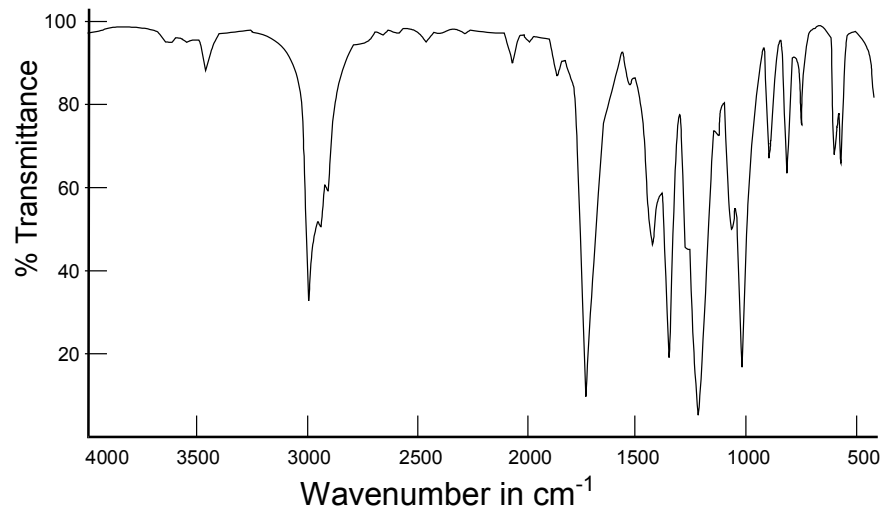
Ultra-violet spectrum

$\lambda = 209 \text{ nm}$, $\epsilon = 72$

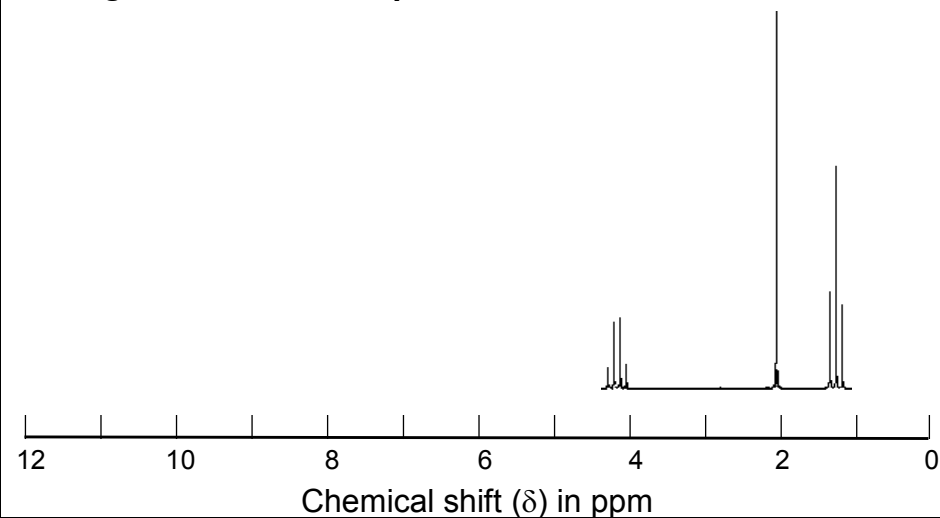
Analysis

Carbon	54.5%	Oxygen	36.4%
Hydrogen	9.1%		

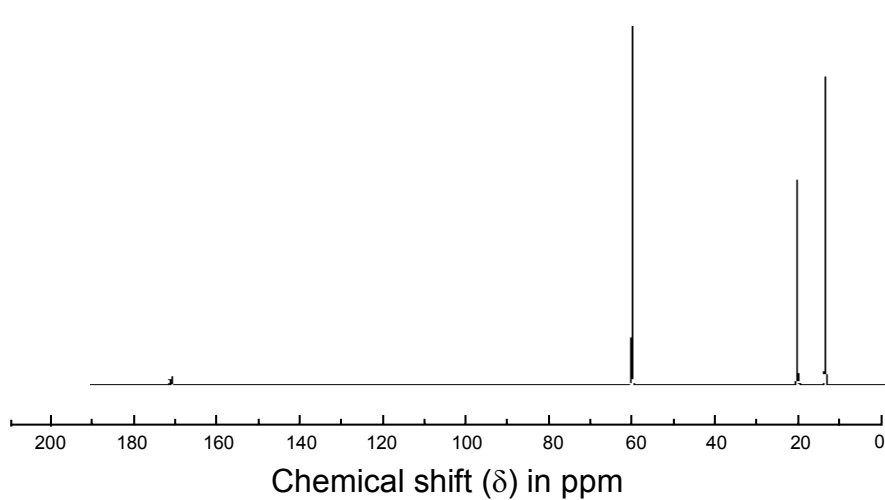
Infra-red spectrum



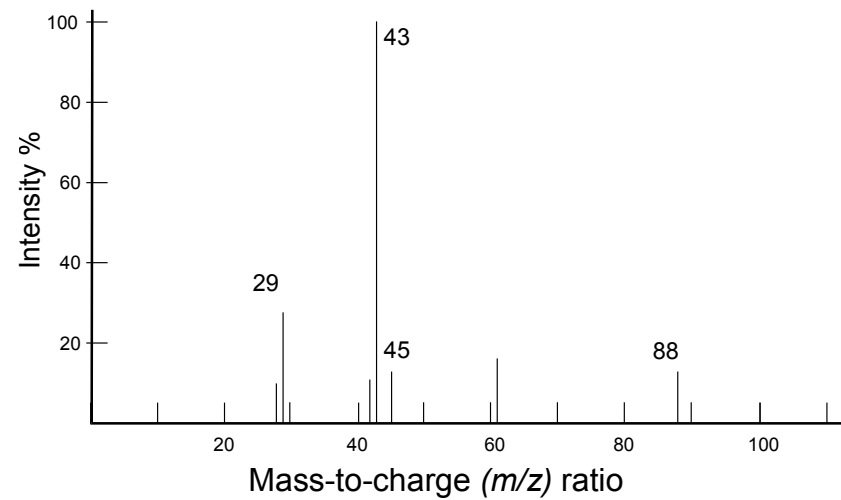
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 22

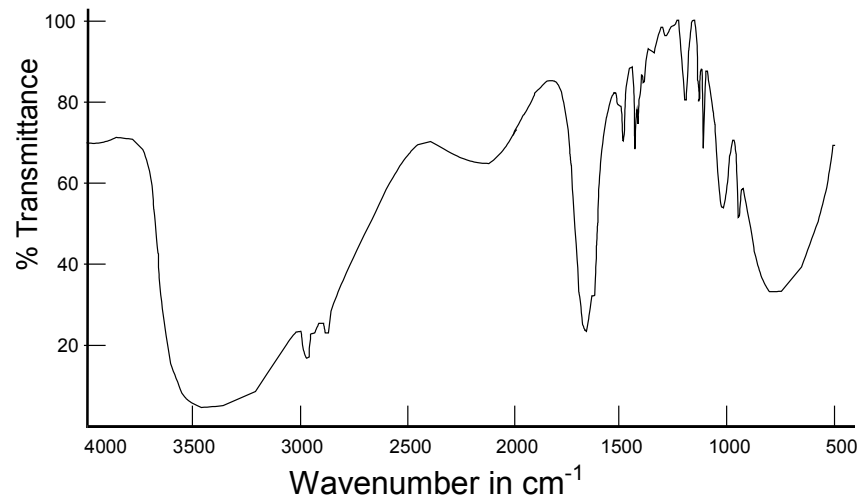
Ultra-violet spectrum

$\lambda = 177 \text{ nm}$, $\varepsilon = 1585$

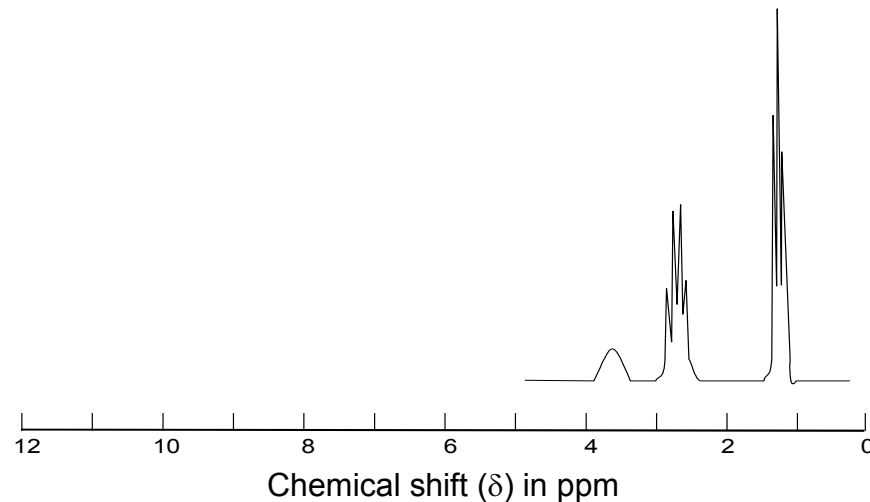
Analysis

Carbon	53.3%	Nitrogen	31.1%
Hydrogen	15.6%		

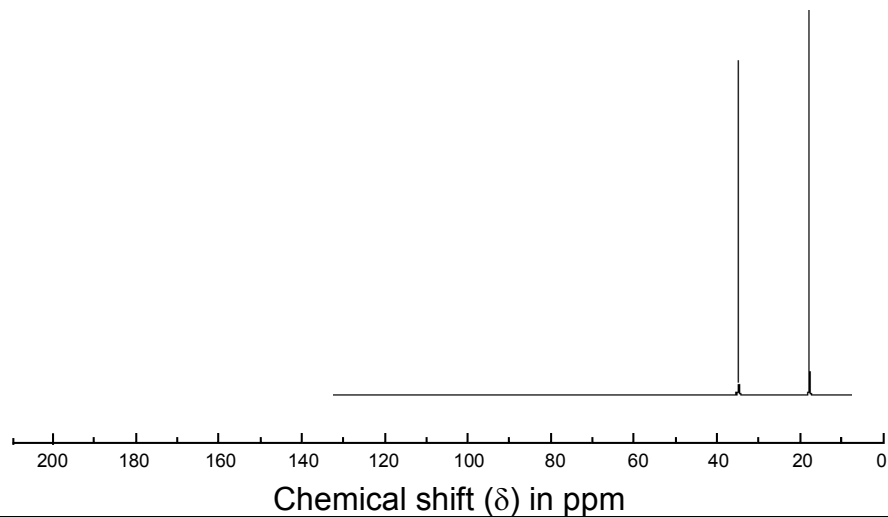
Infra-red spectrum



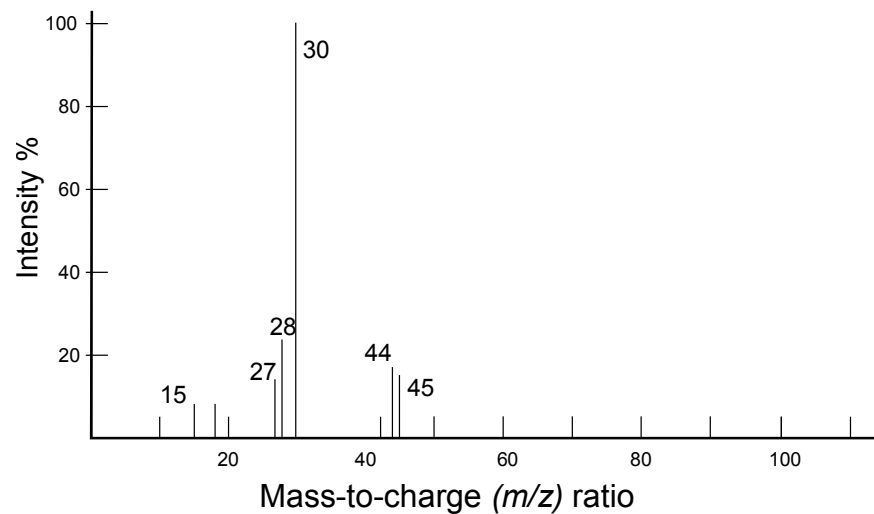
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 23

Ultra-violet spectrum

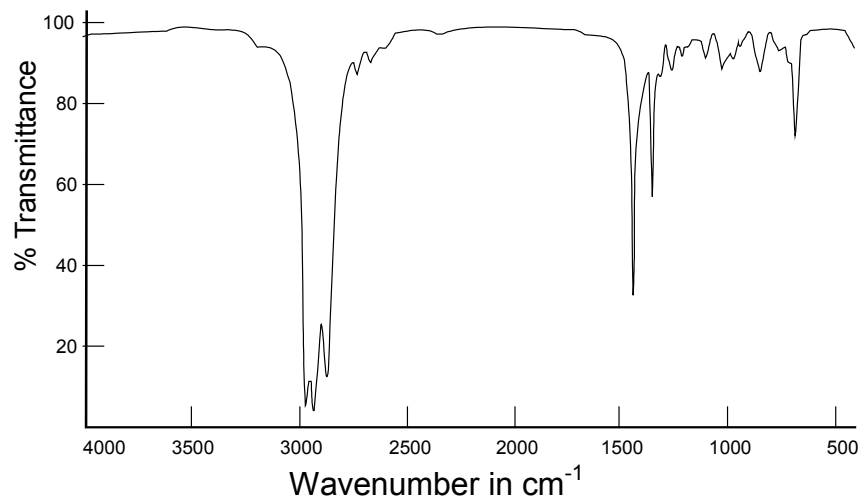
No data available

Analysis

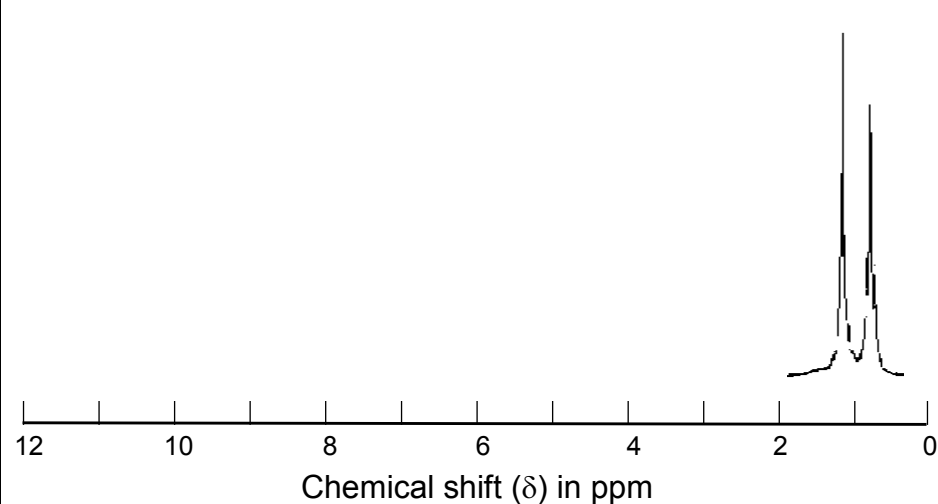
Carbon 83.7%

Hydrogen 16.3%

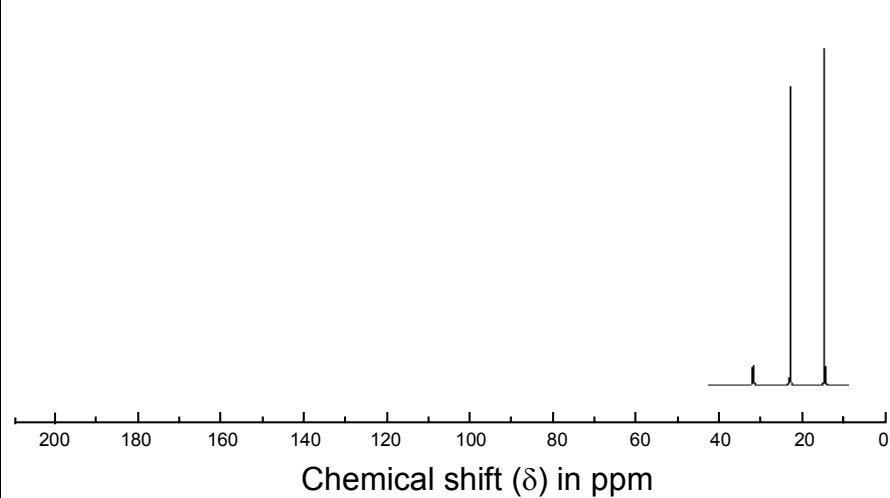
Infra-red spectrum



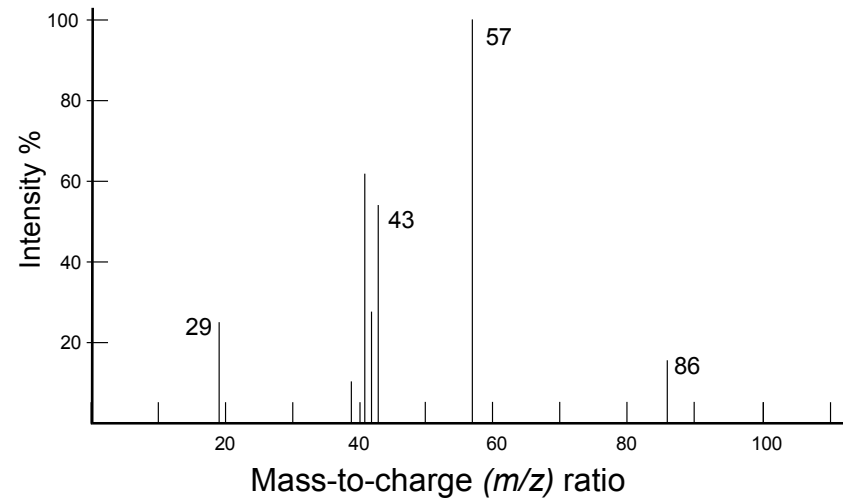
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 24

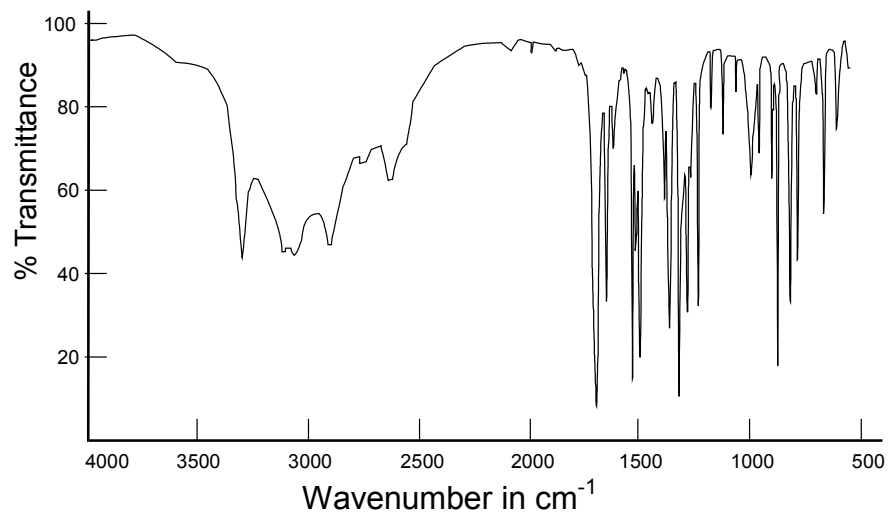
Ultra-violet spectrum

$\lambda = 254 \text{ nm}$, $\epsilon = 15100$

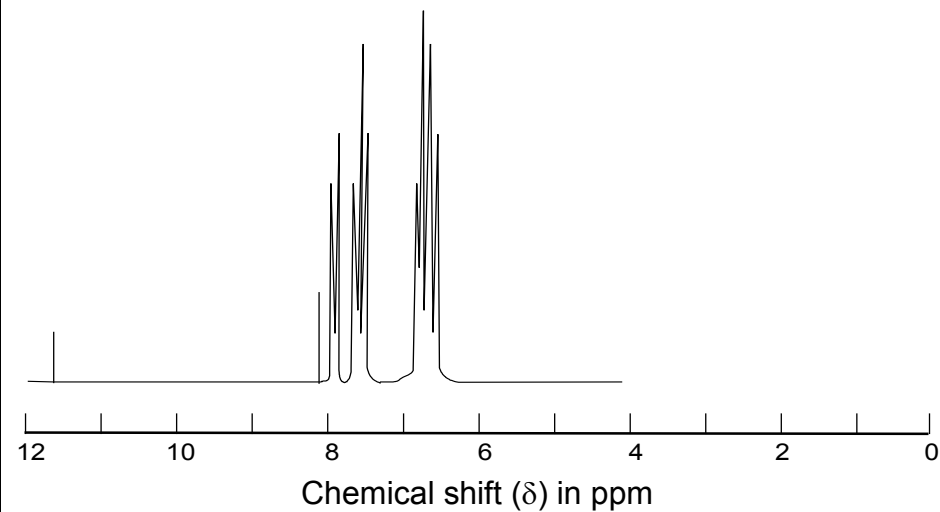
Analysis

Carbon	60.9%	Oxygen	34.8%
Hydrogen	4.3%		

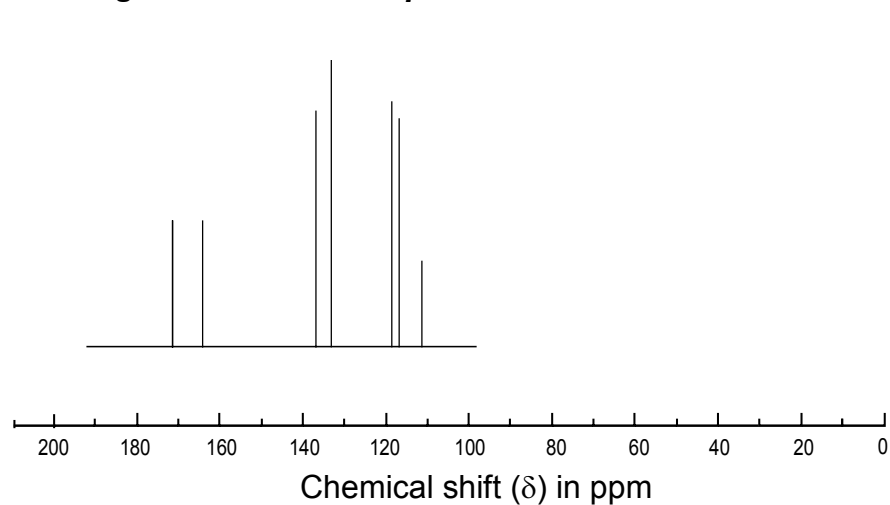
Infra-red spectrum



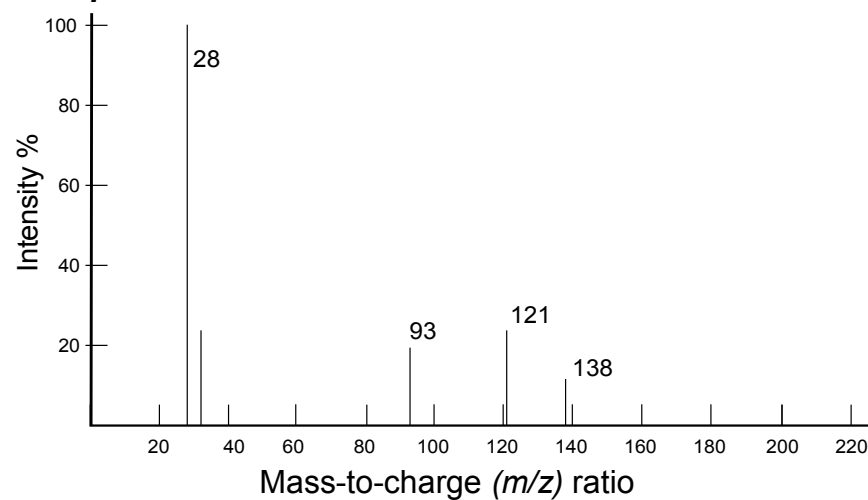
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 25

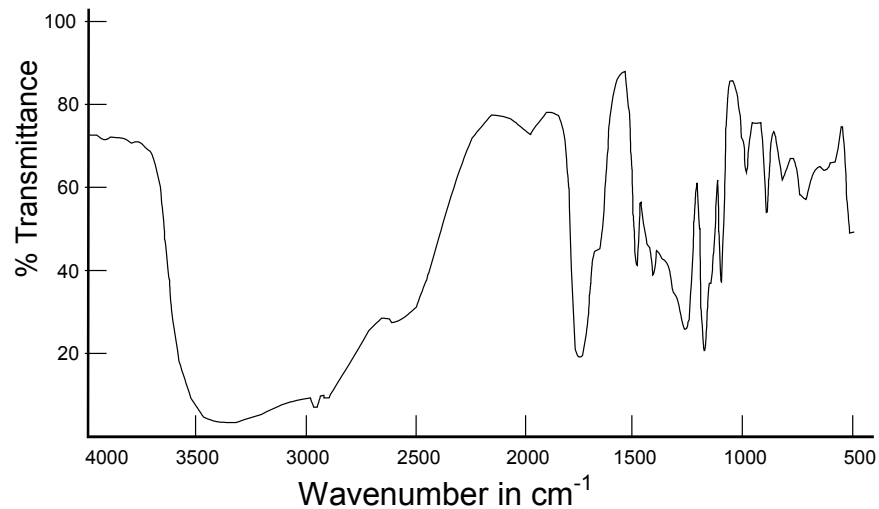
Ultra-violet spectrum

No data available

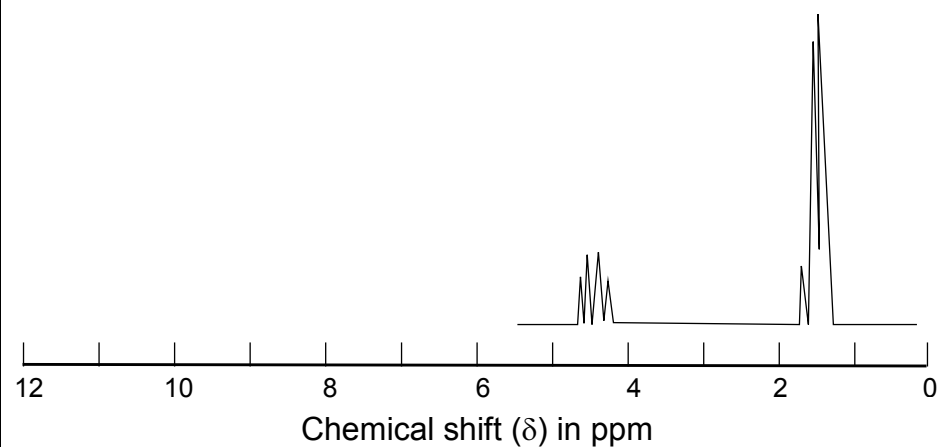
Analysis

Carbon	40.0%	Oxygen	53.3%
Hydrogen	6.7%		

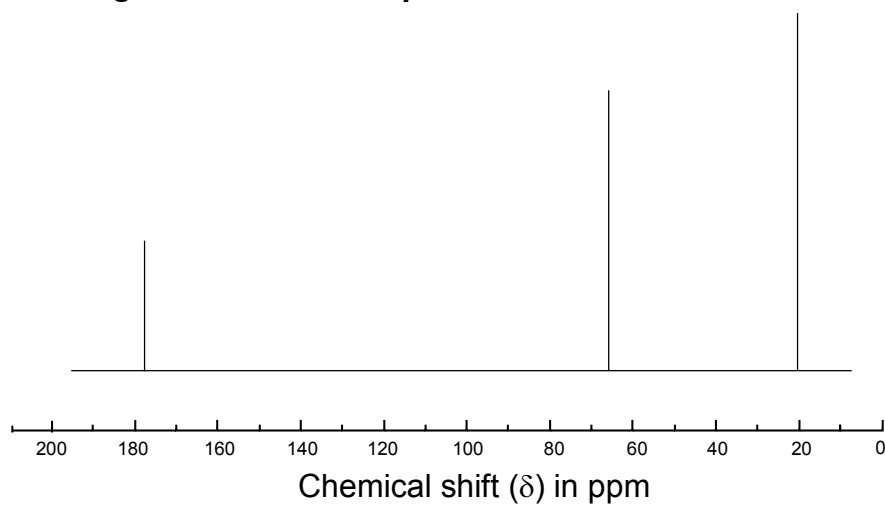
Infra-red spectrum



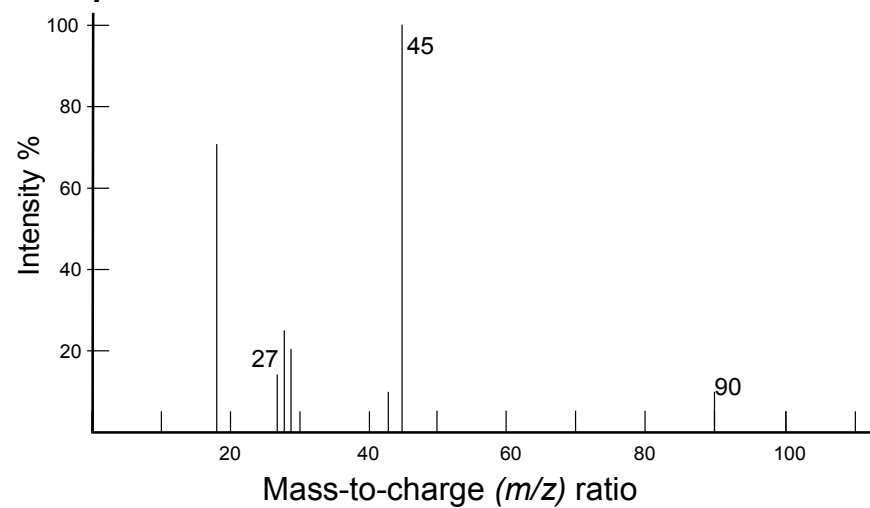
¹H magnetic resonance spectrum



¹³C magnetic resonance spectrum



Mass spectrum



Substance 26

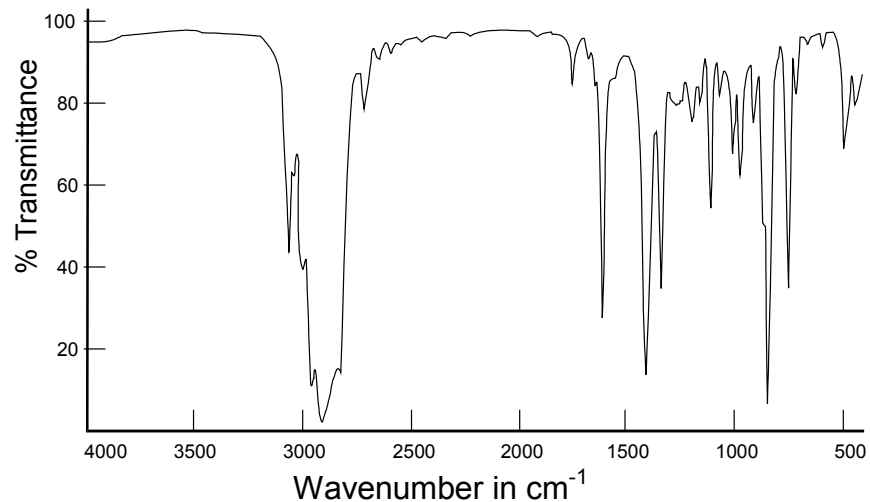
Ultra-violet spectrum

$\lambda = 220 \text{ nm}$, $\epsilon = 257$

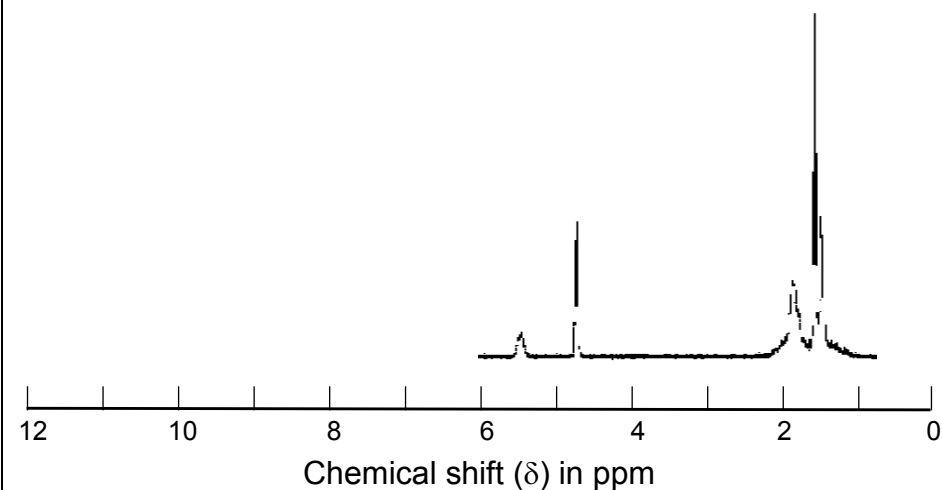
Analysis

Carbon 88.2%
Hydrogen 11.8%

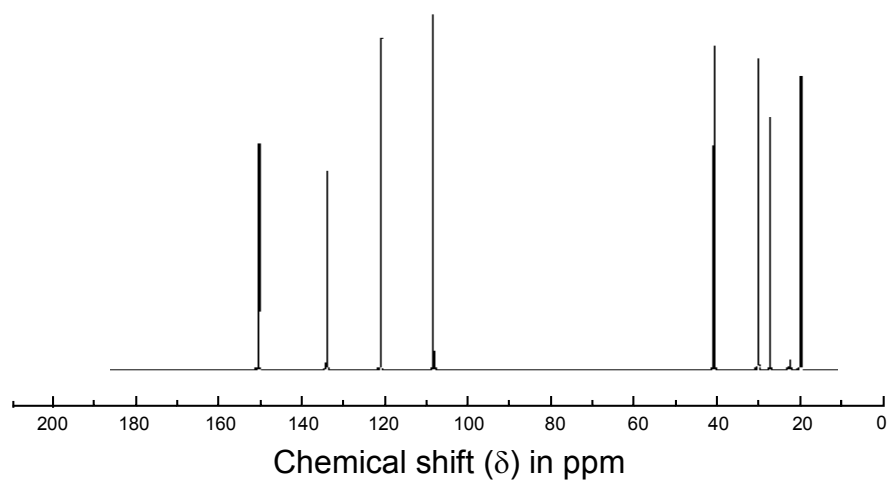
Infra-red spectrum



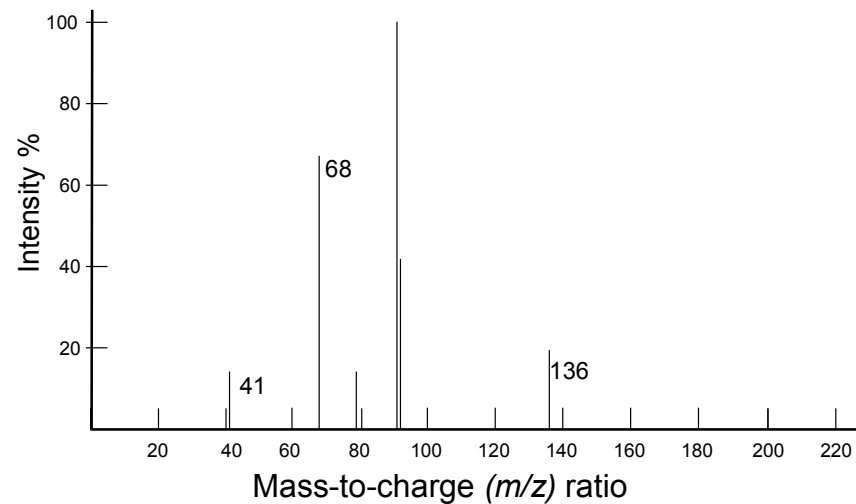
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 27

Ultra-violet spectrum

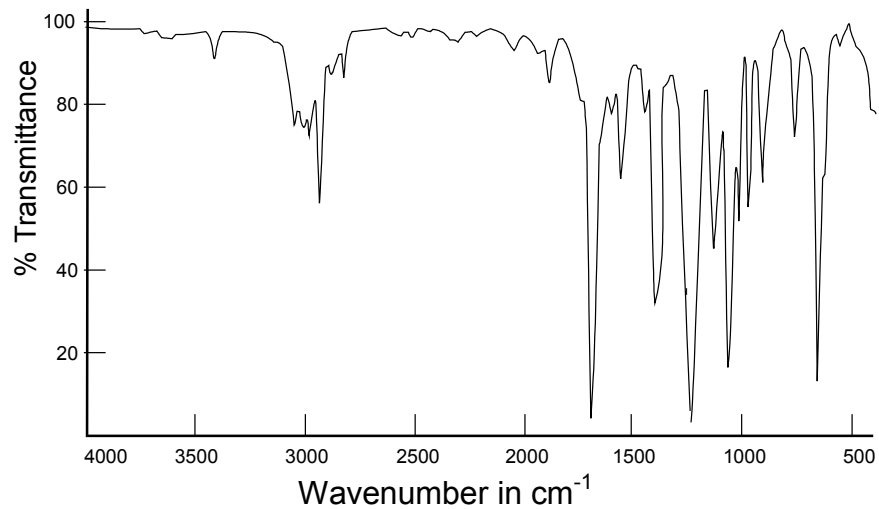
$\lambda = 280 \text{ nm}$, $\epsilon = 686$

$\lambda = 228 \text{ nm}$, $\epsilon = 11000$

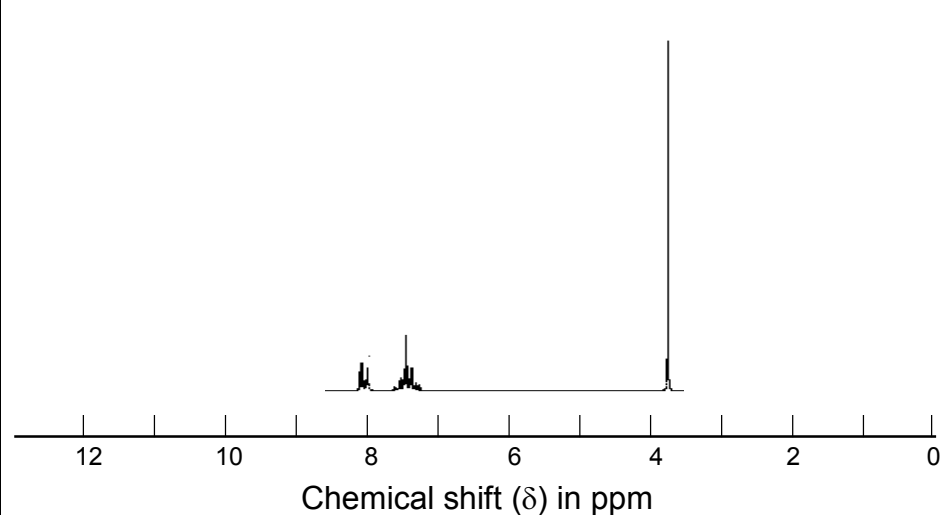
Analysis

Carbon	70.6%	Oxygen	23.5%
Hydrogen	5.9%		

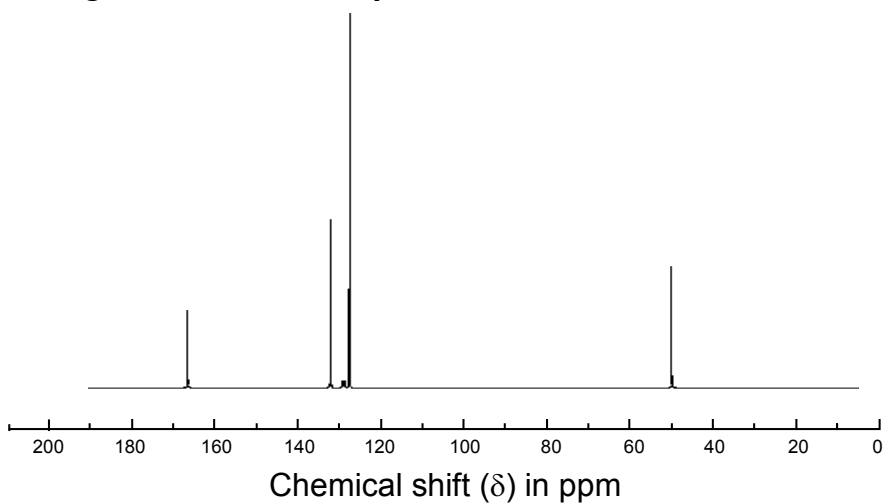
Infra-red spectrum



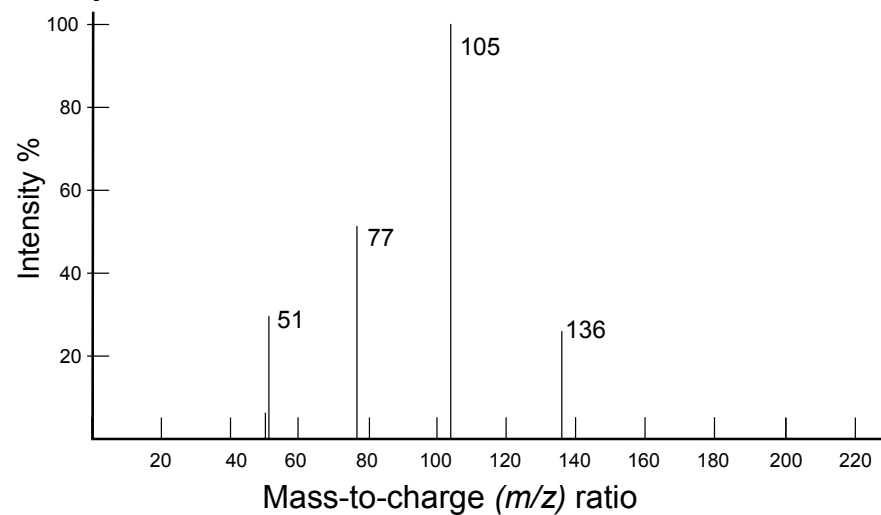
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 28

Ultra-violet spectrum

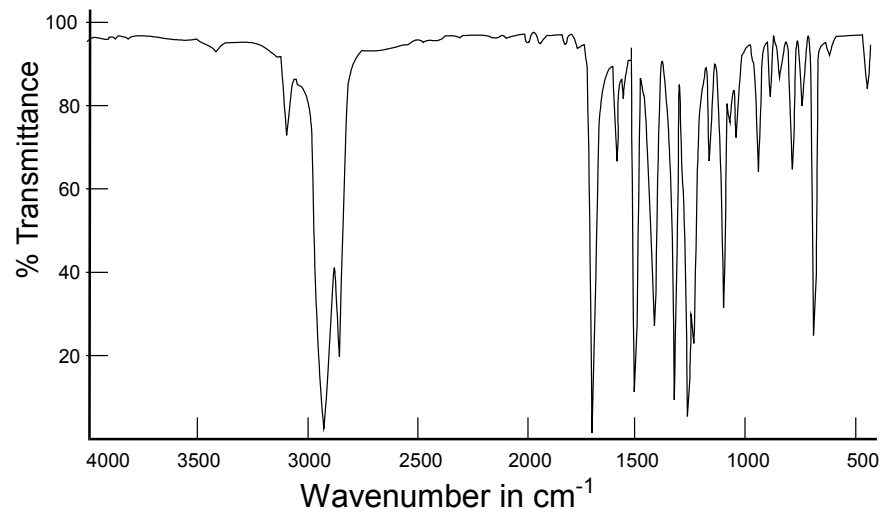
$\lambda = 255 \text{ nm}$, $\epsilon = 7360$

$\lambda = 217 \text{ nm}$, $\epsilon = 26200$

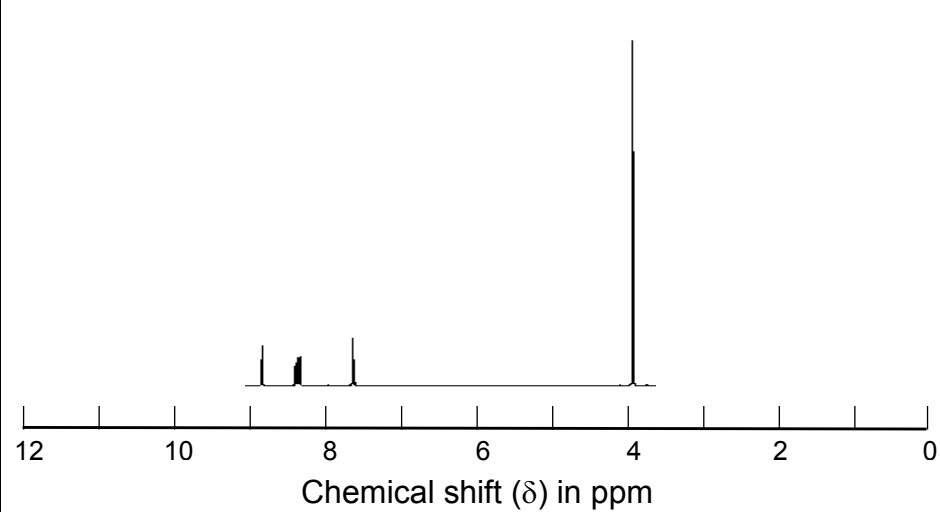
Analysis

Carbon	53.0%	Oxygen	35.3%
Hydrogen	3.9%	Nitrogen	7.7%

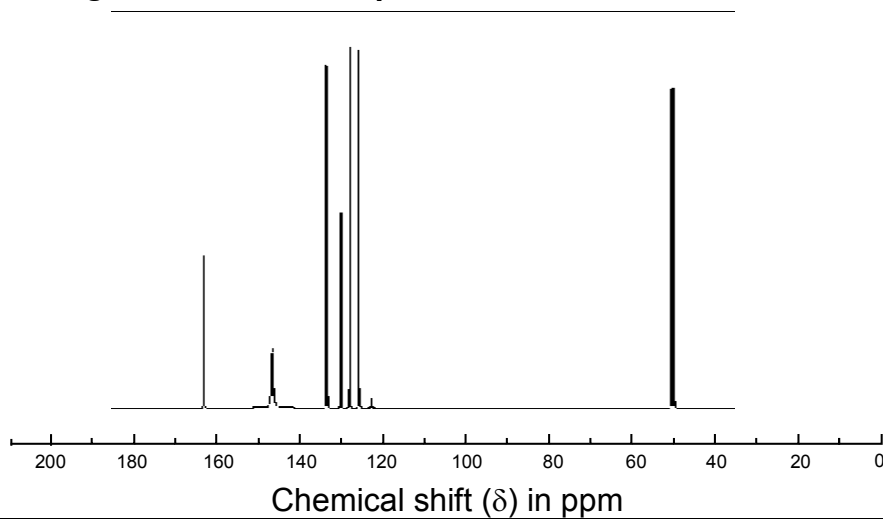
Infra-red spectrum



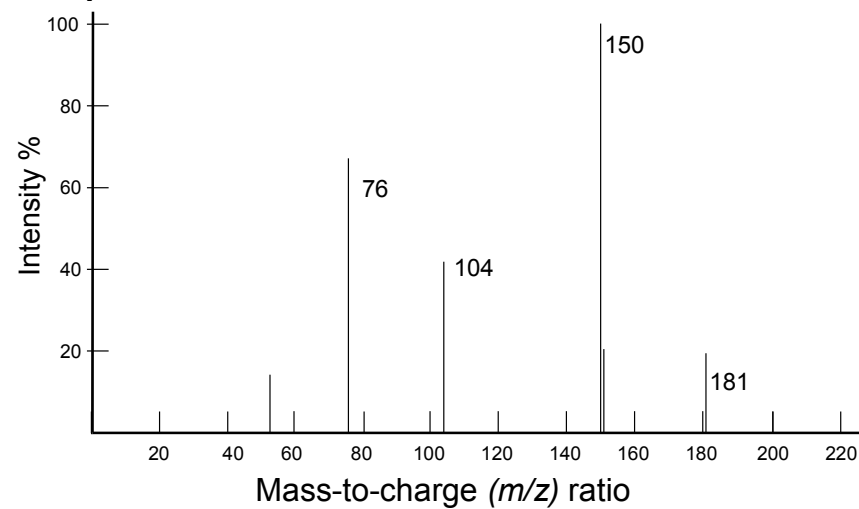
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 29

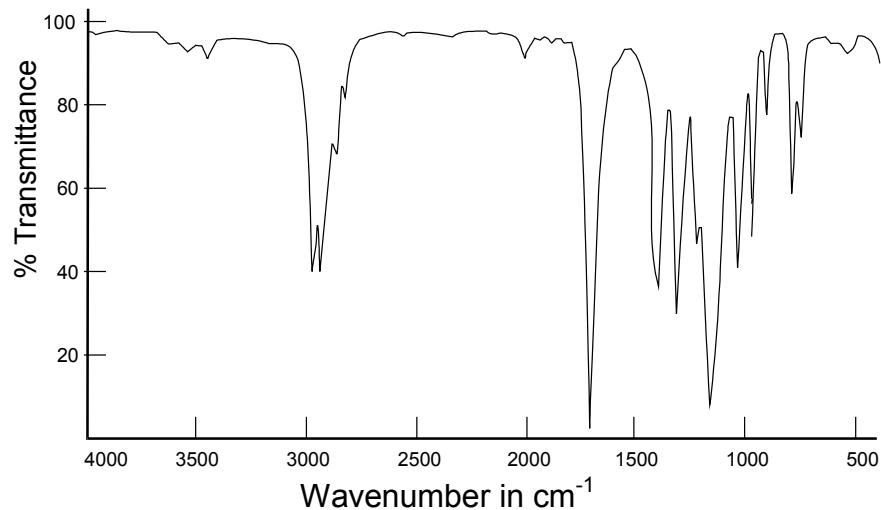
Ultra-violet spectrum

$\lambda = 211 \text{ nm}$, $\epsilon = 62$

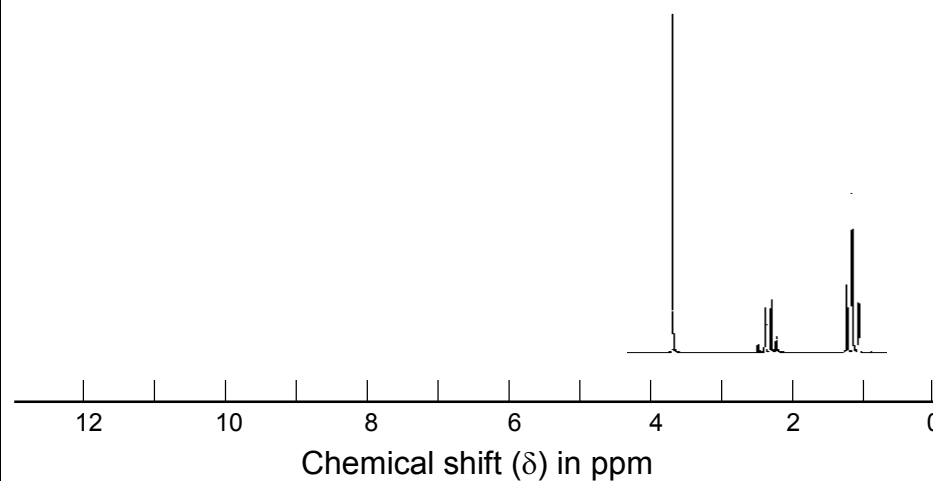
Analysis

Carbon	54.5%	Oxygen	36.4%
Hydrogen	9.1%		

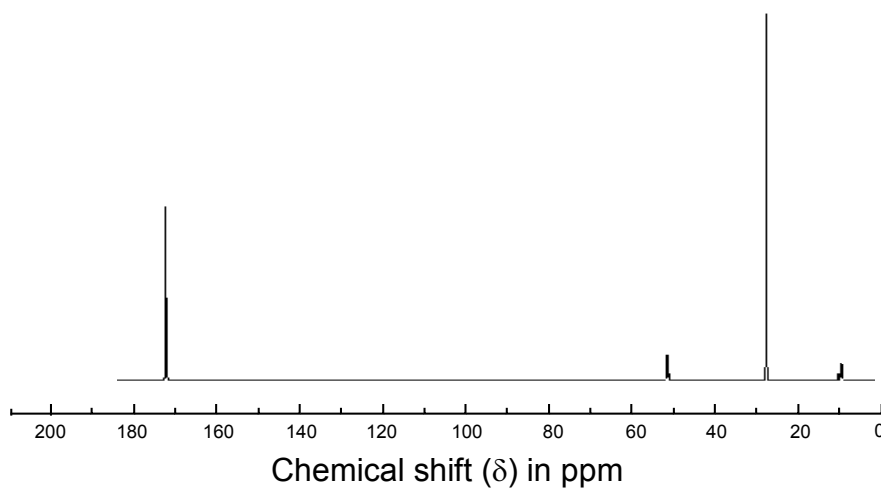
Infra-red spectrum



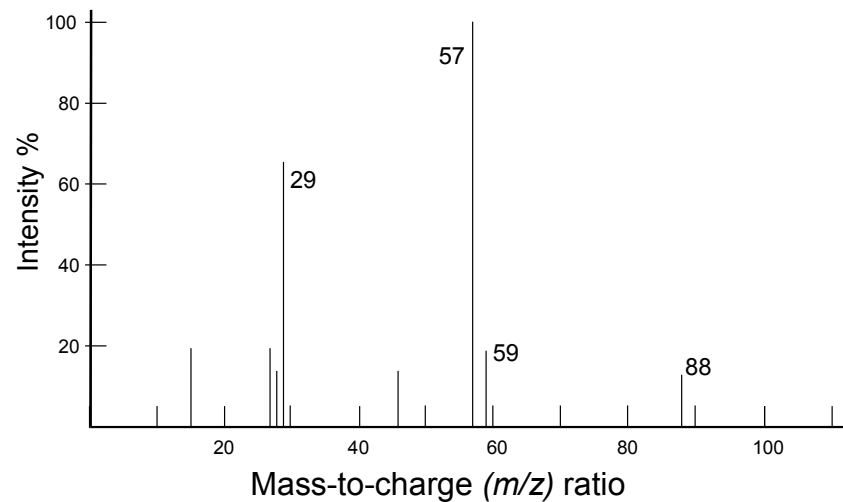
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 30

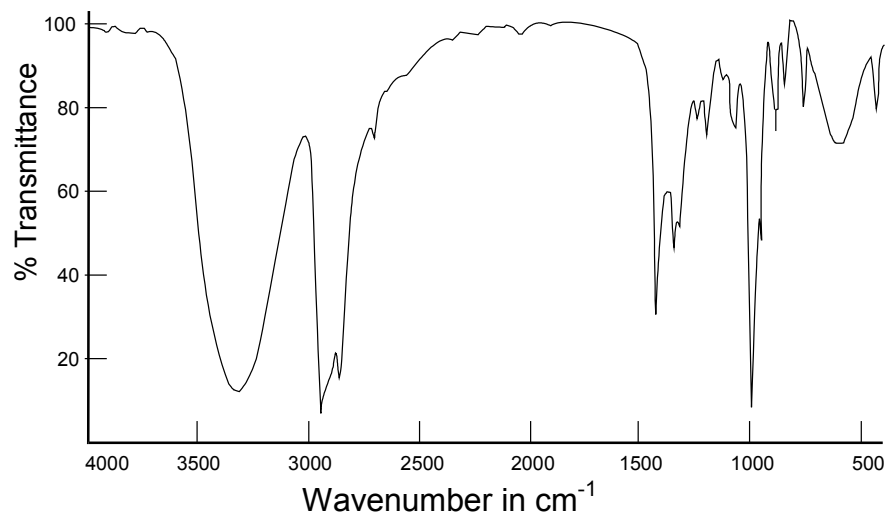
Ultra-violet spectrum

No data available

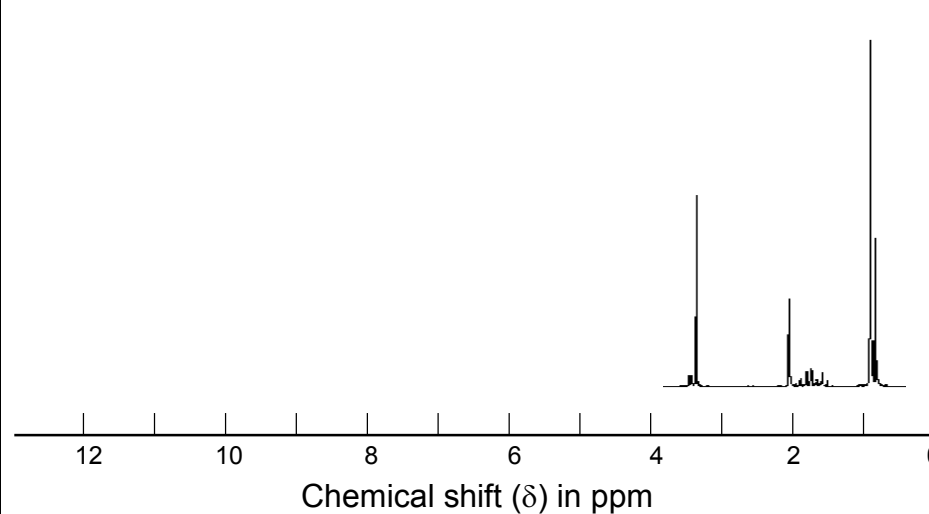
Analysis

Carbon	64.9%	Oxygen	21.6%
Hydrogen	13.5%		

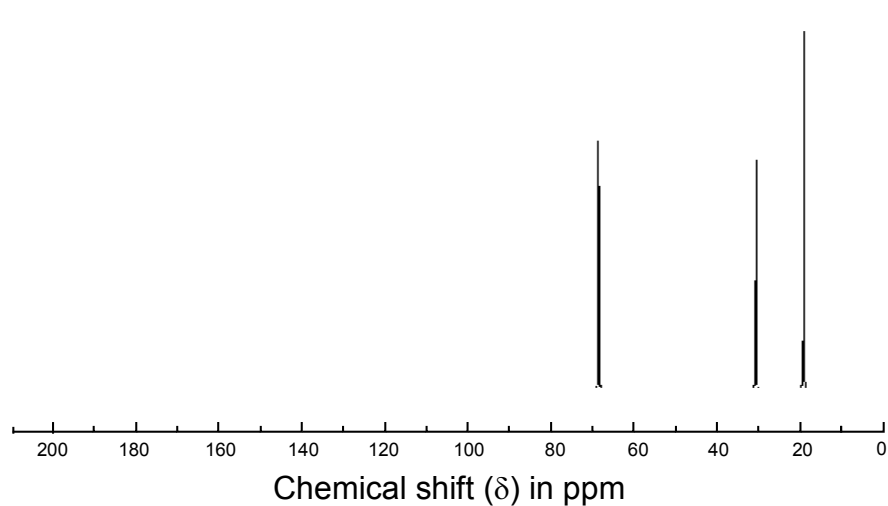
Infra-red spectrum



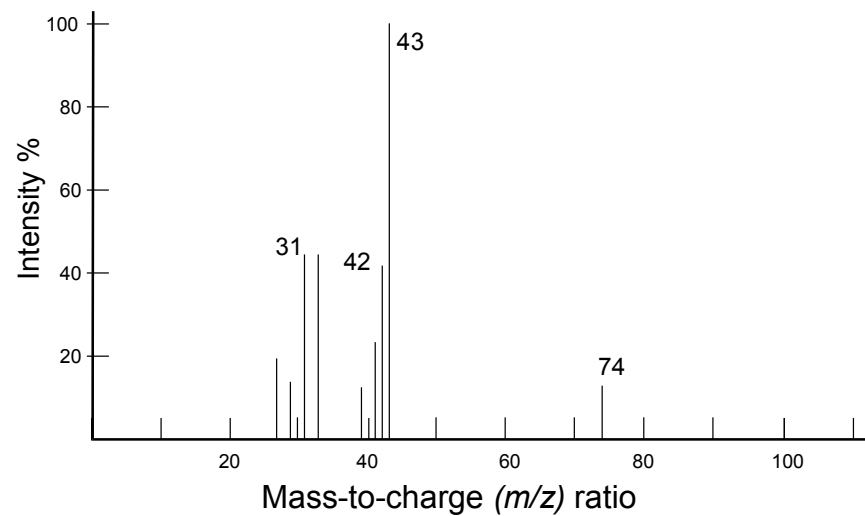
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 31

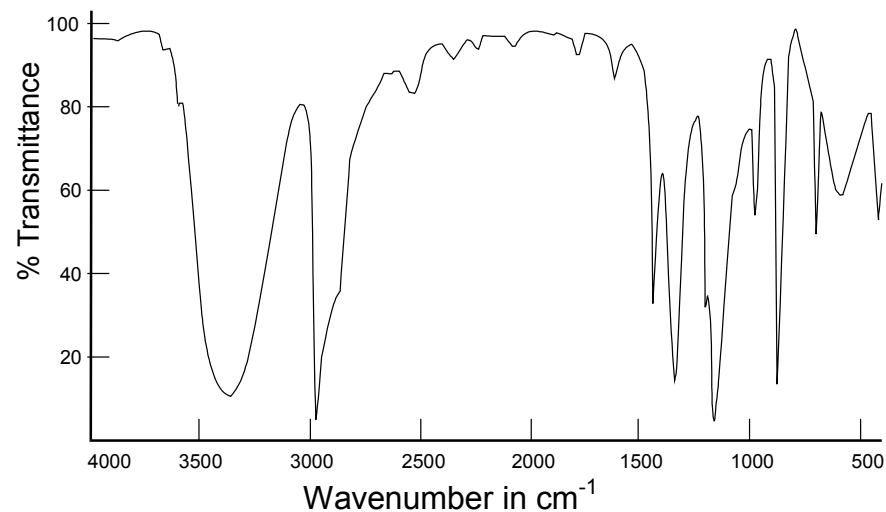
Ultra-violet spectrum

$\lambda = 300 \text{ nm}$, $\epsilon = 1349$

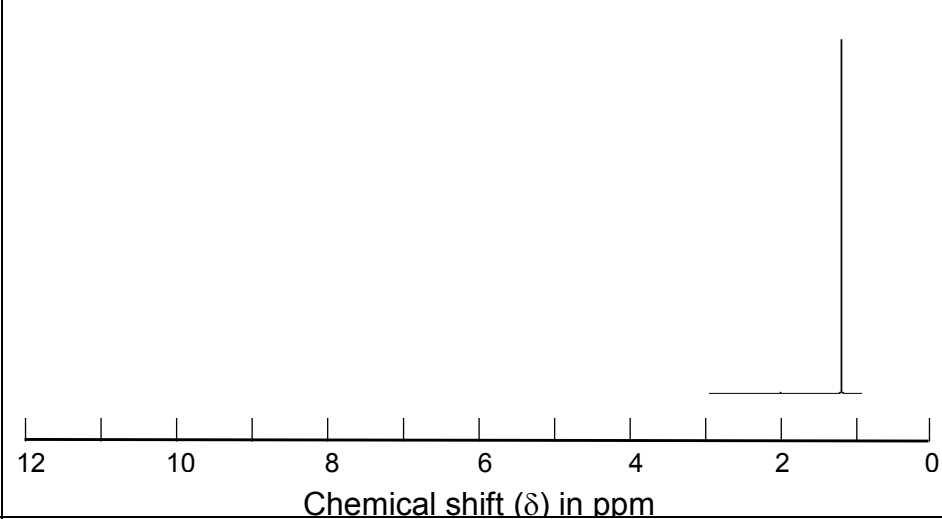
Analysis

Carbon	64.9%	Oxygen	21.6%
Hydrogen	13.5%		

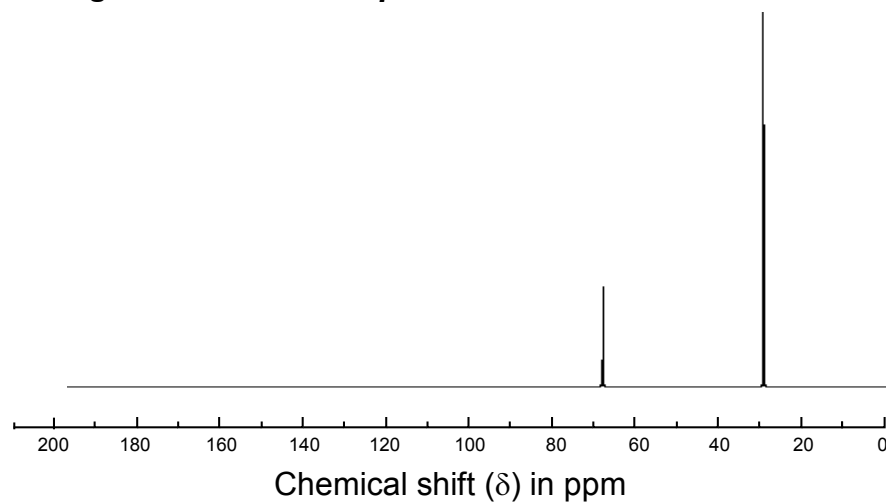
Infra-red spectrum



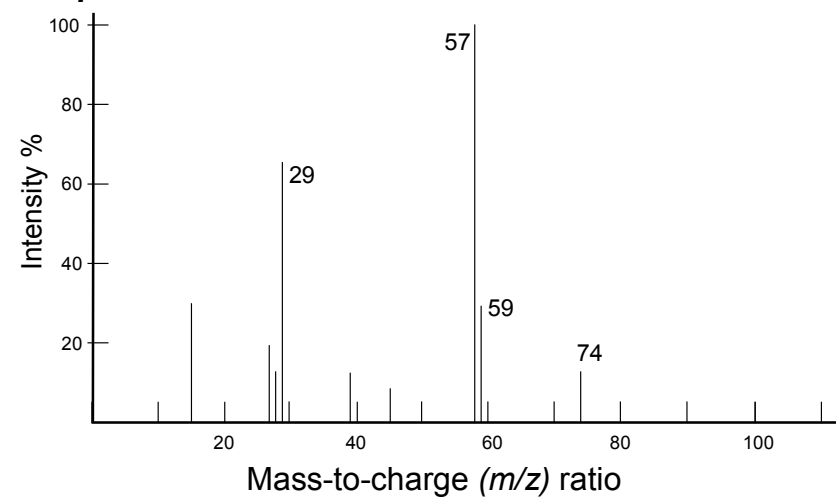
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 32

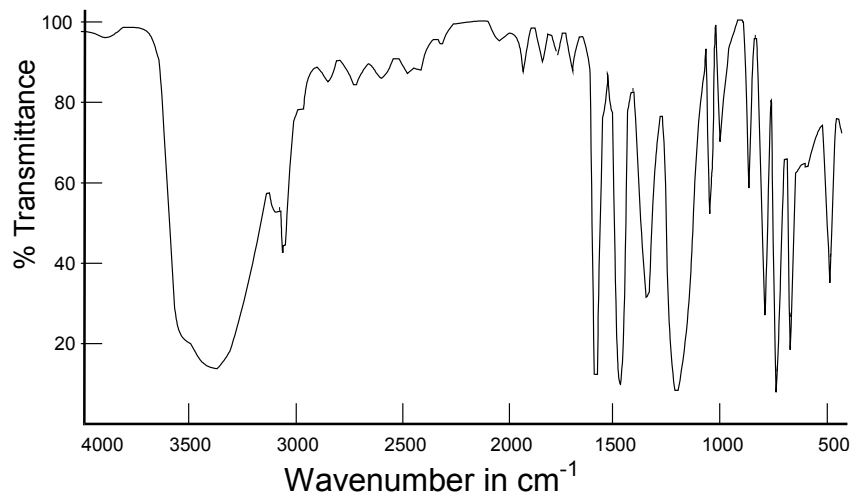
Ultra-violet spectrum

$\lambda = 277 \text{ nm}$, $\epsilon = \text{no data}$

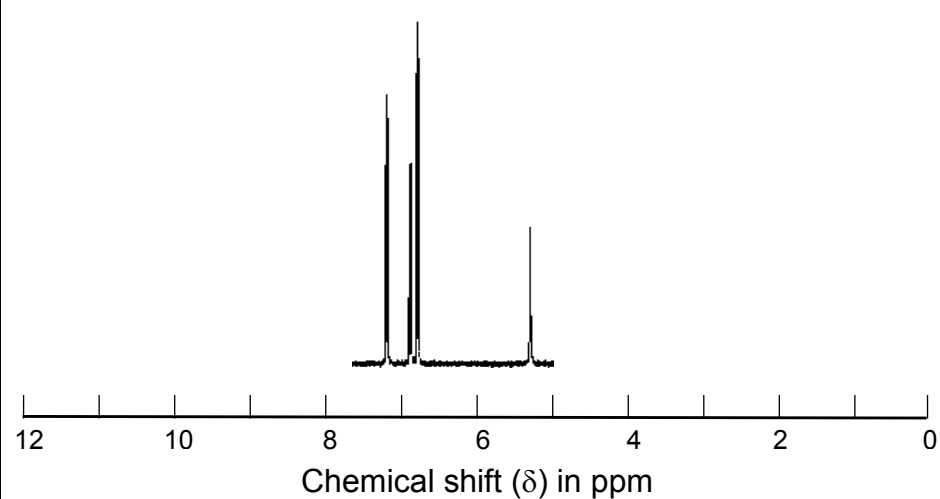
Analysis

Carbon	76.7%	Oxygen	17.0%
Hydrogen	6.4%		

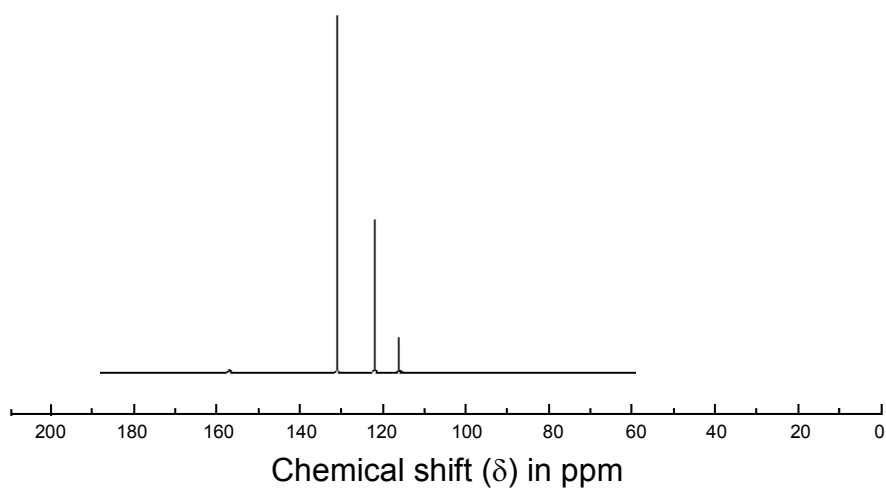
Infra-red spectrum



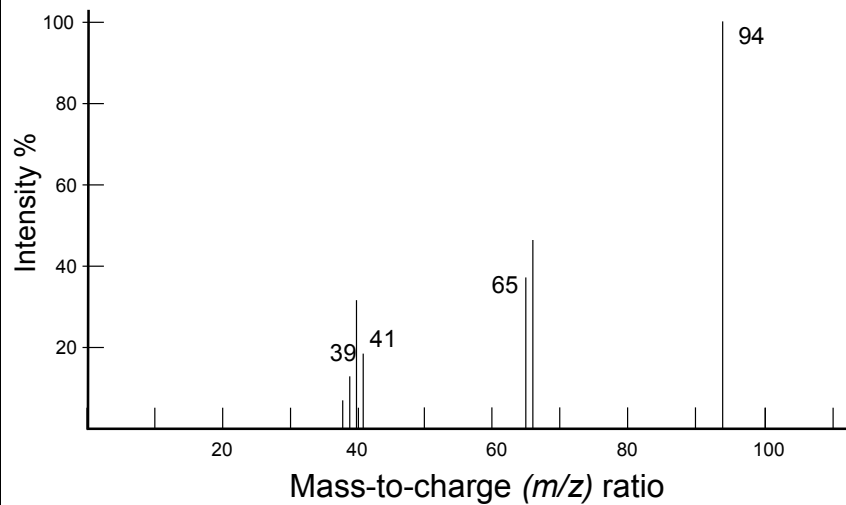
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 33

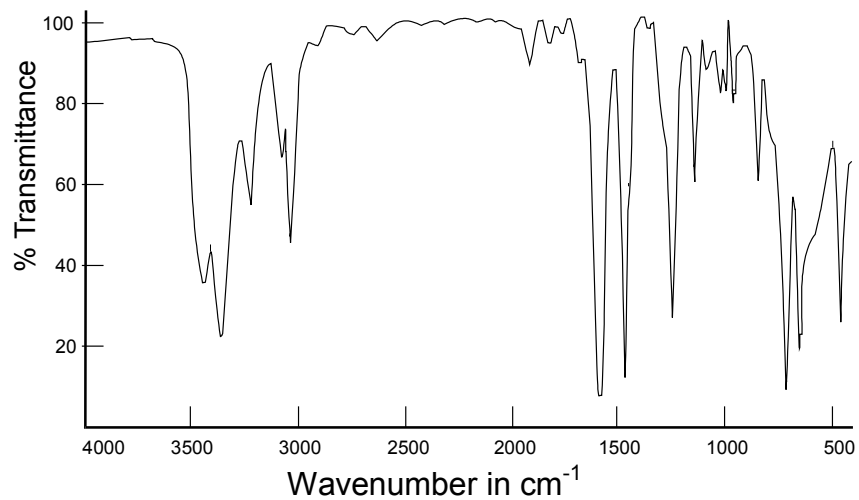
Ultra-violet spectrum

$\lambda = 287 \text{ nm}$, $\epsilon = \text{no data}$

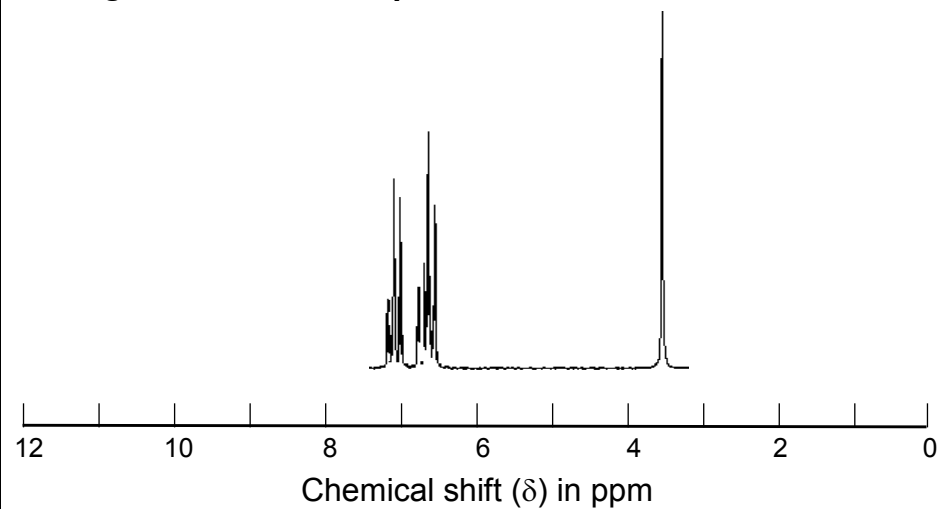
Analysis

Carbon	77.4%	Oxygen	15.1%
Hydrogen	7.5%		

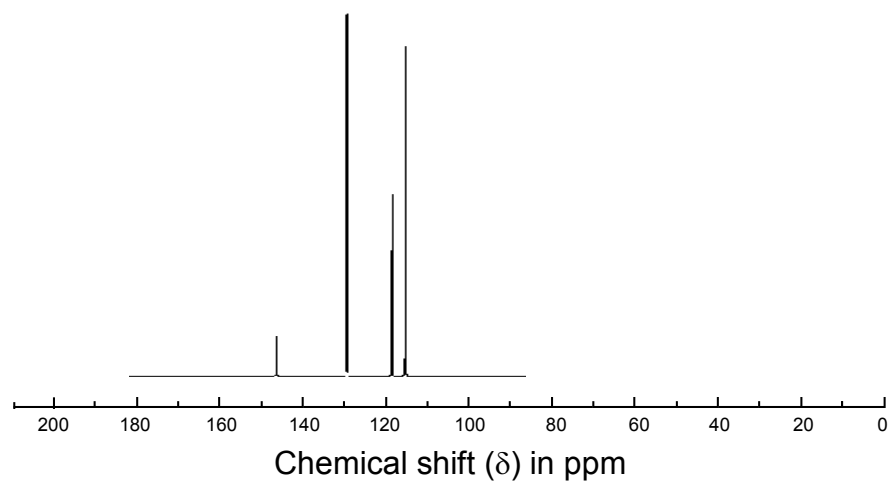
Infra-red spectrum



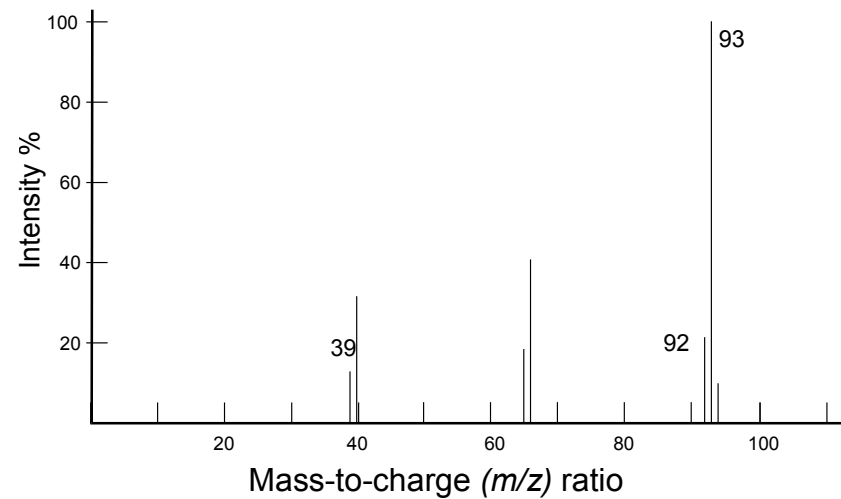
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum

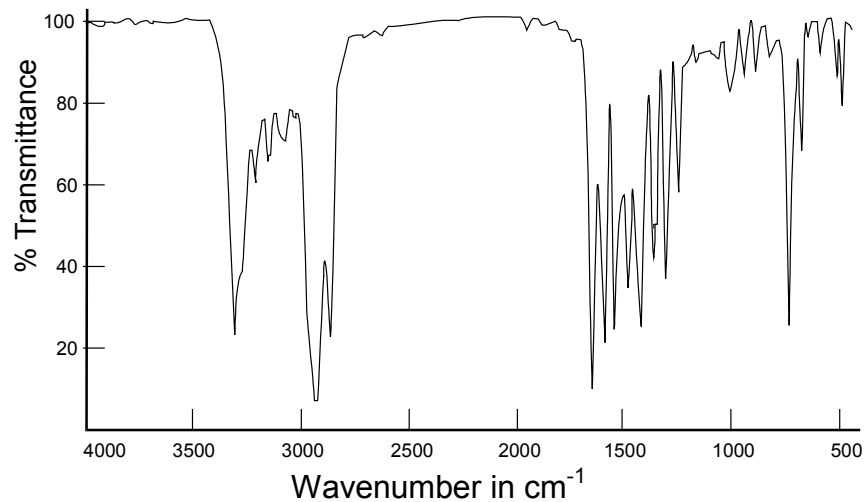
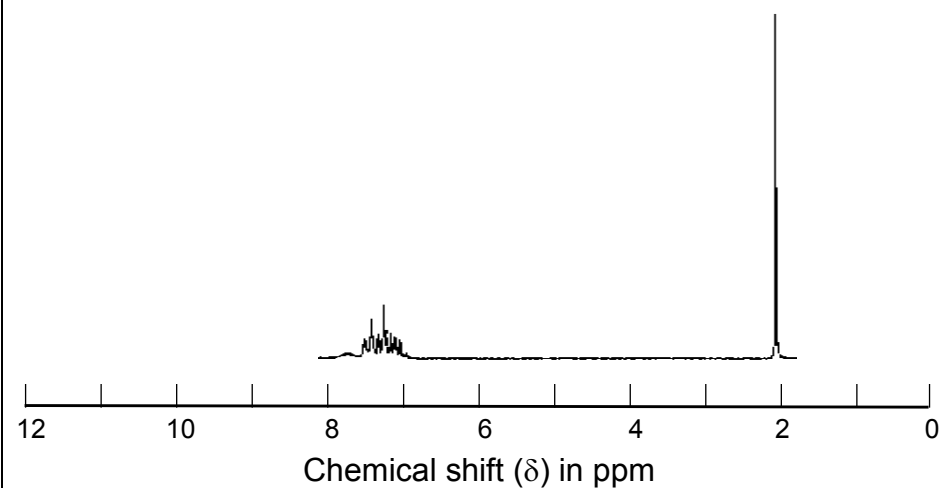
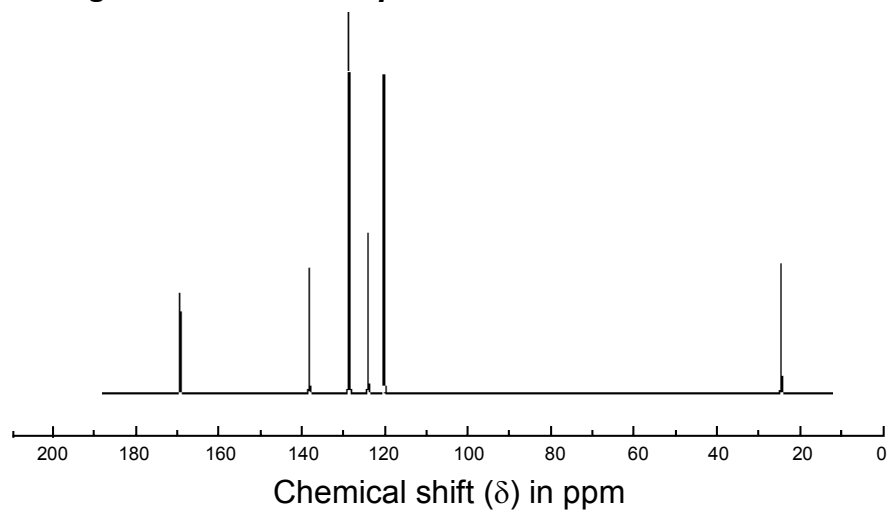
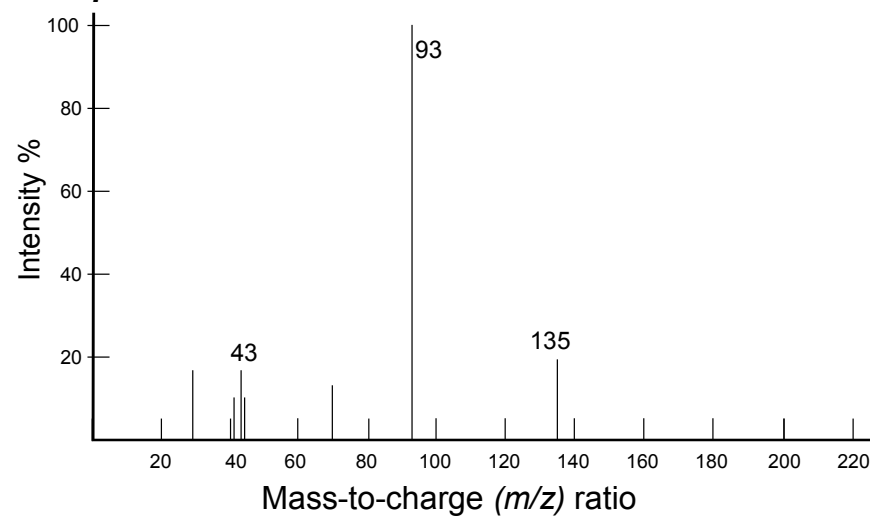


Mass spectrum



Substance 34**Ultra-violet spectrum** $\lambda = 241 \text{ nm}$, $\epsilon = \text{no data}$ **Analysis**

Carbon	71.1%	Oxygen	11.9%
Hydrogen	6.7%	Nitrogen	10.4%

Infra-red spectrum **^1H magnetic resonance spectrum** **^{13}C magnetic resonance spectrum****Mass spectrum**

Substance 35

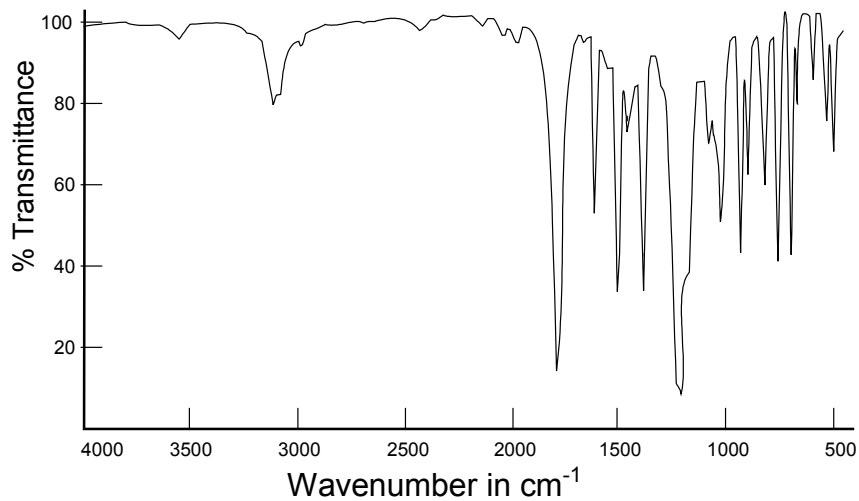
Ultra-violet spectrum

$\lambda = 260 \text{ nm}$, $\epsilon = 302$

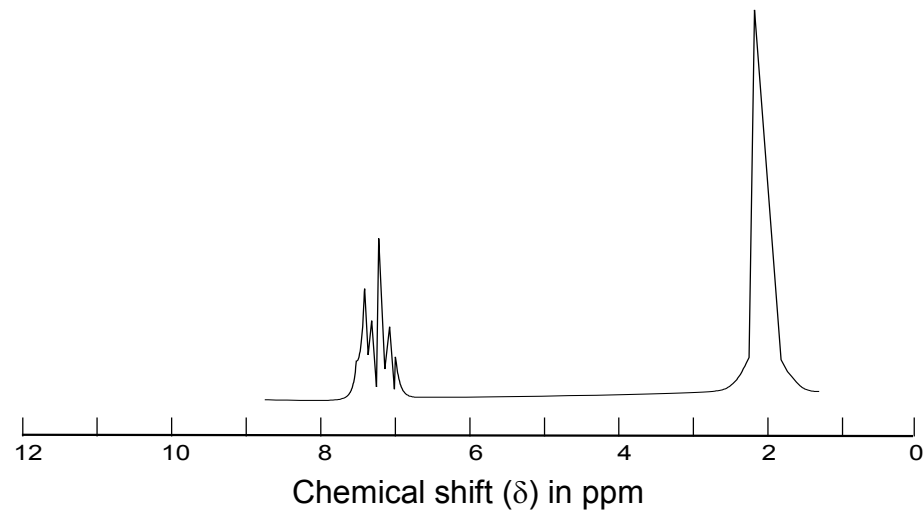
Analysis

Carbon	70.6%	Oxygen	23.5%
Hydrogen	5.9%		

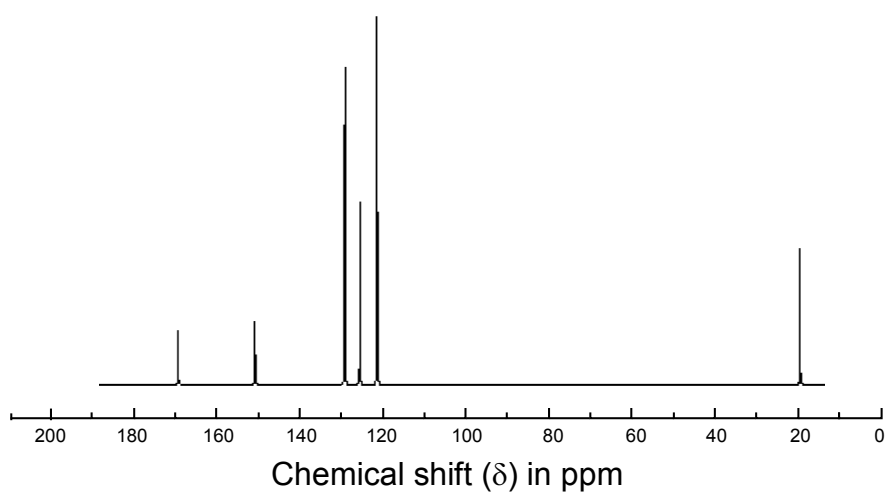
Infra-red spectrum



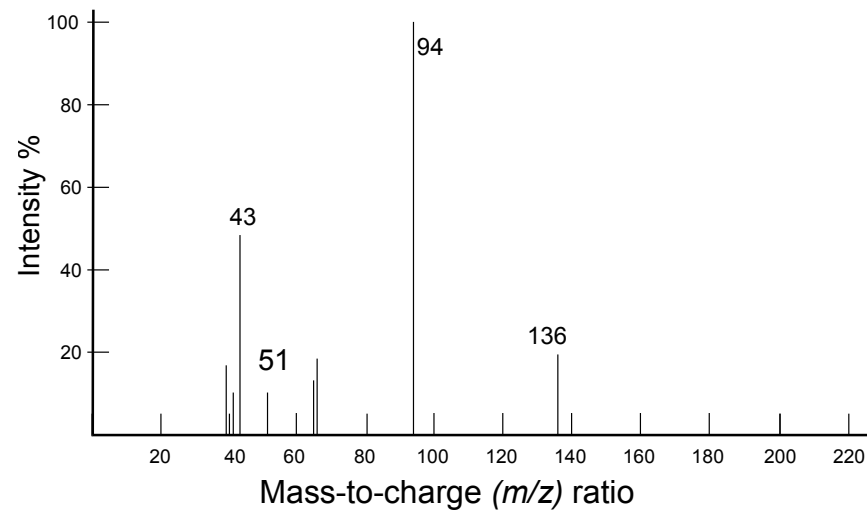
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 36

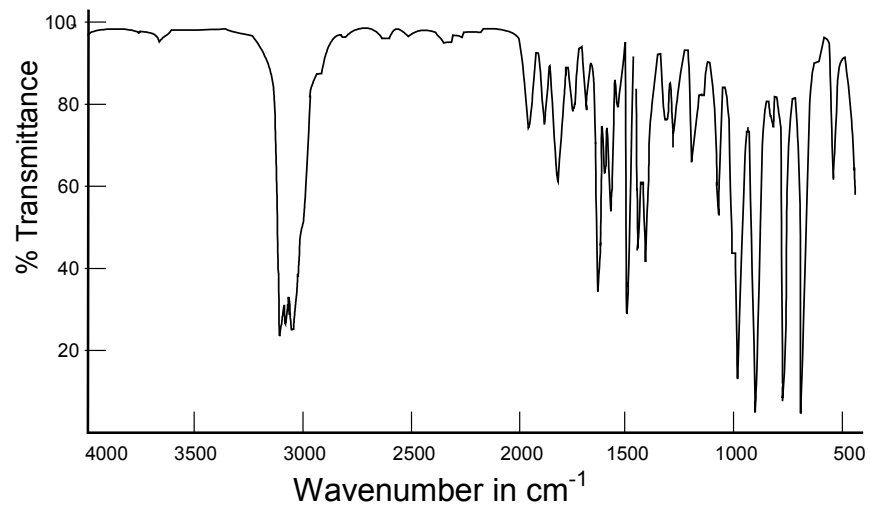
Ultra-violet spectrum

$\lambda = 289 \text{ nm}$, $\epsilon = 272$

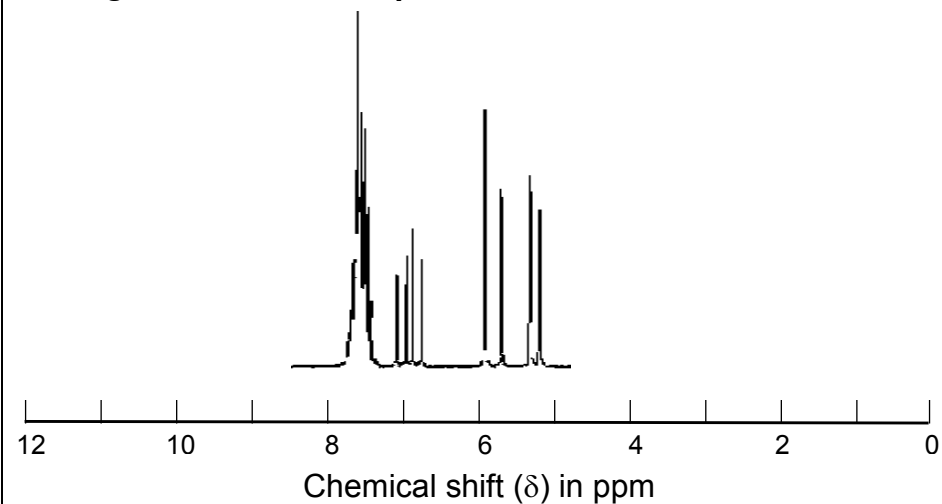
Analysis

Carbon 92.3%
Hydrogen 7.7%

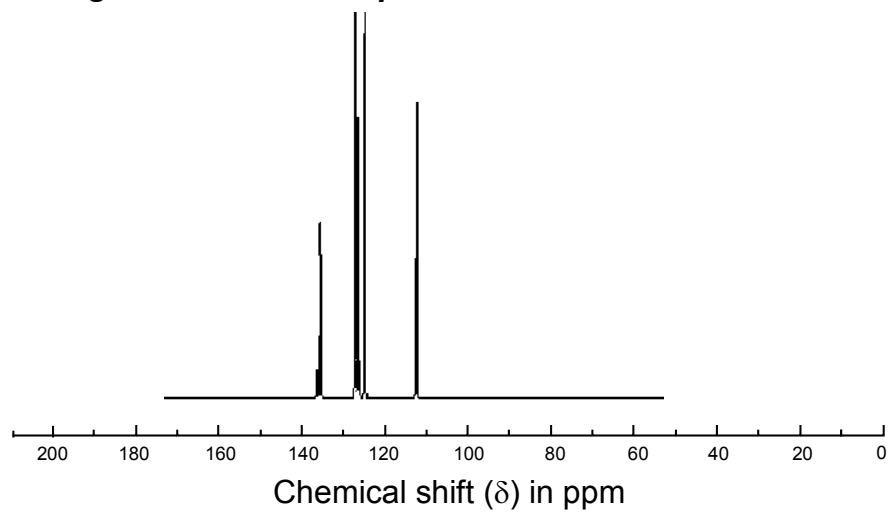
Infra-red spectrum



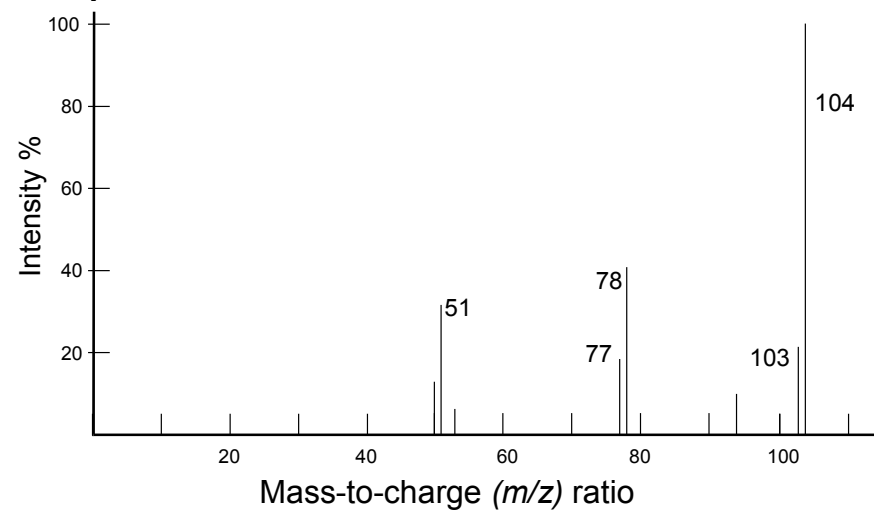
^1H magnetic resonance spectrum



^{13}C magnetic resonance spectrum



Mass spectrum



Substance 37

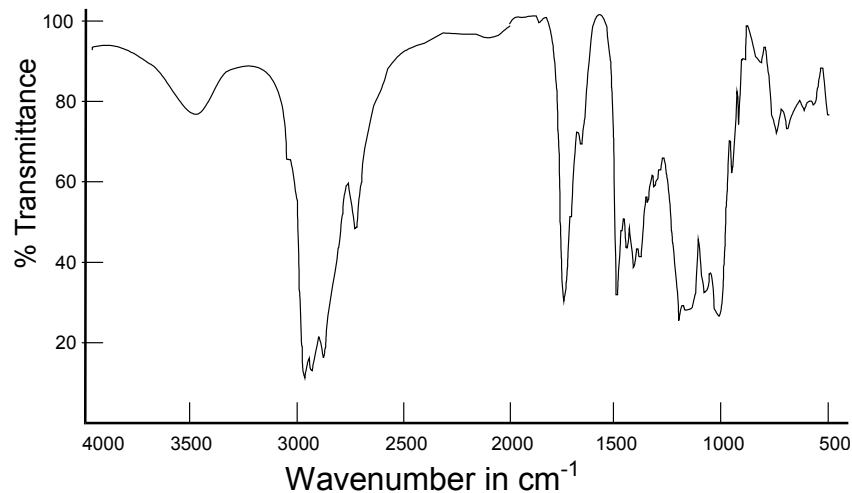
Ultra-violet spectrum

No data available

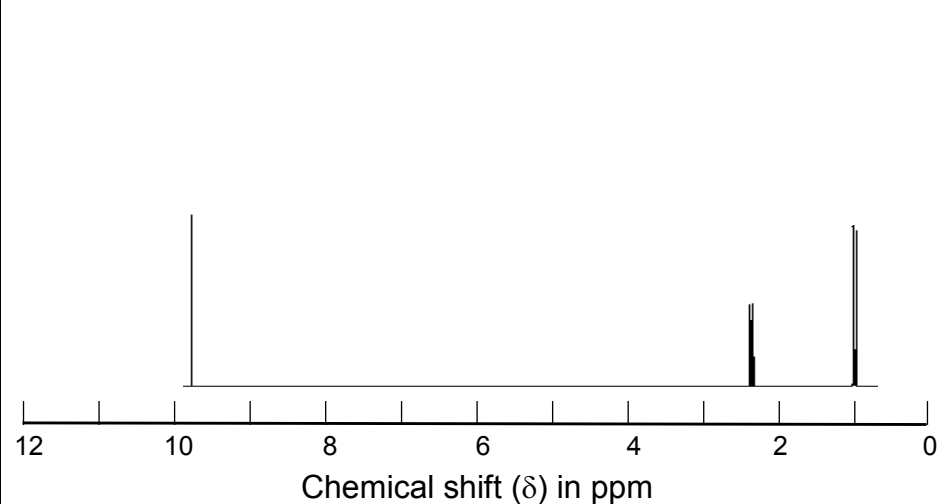
Analysis

Carbon	62.1%	Oxygen	27.6%
Hydrogen	10.3%		

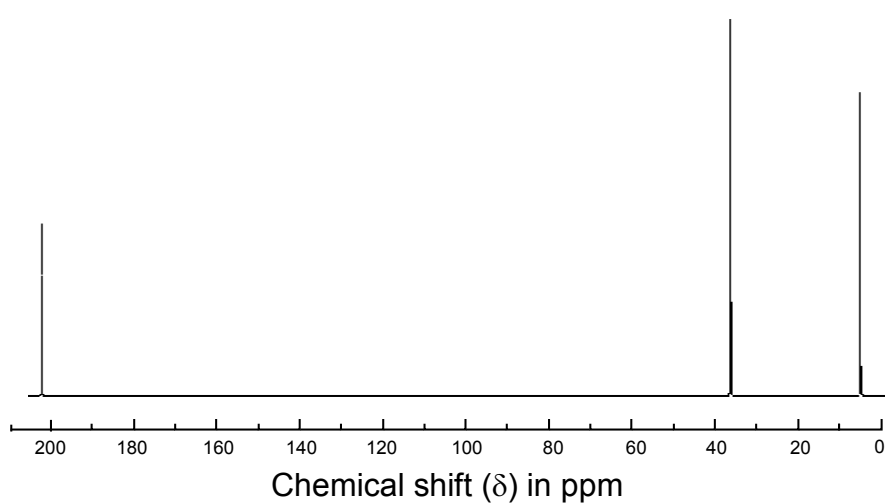
Infra-red spectrum



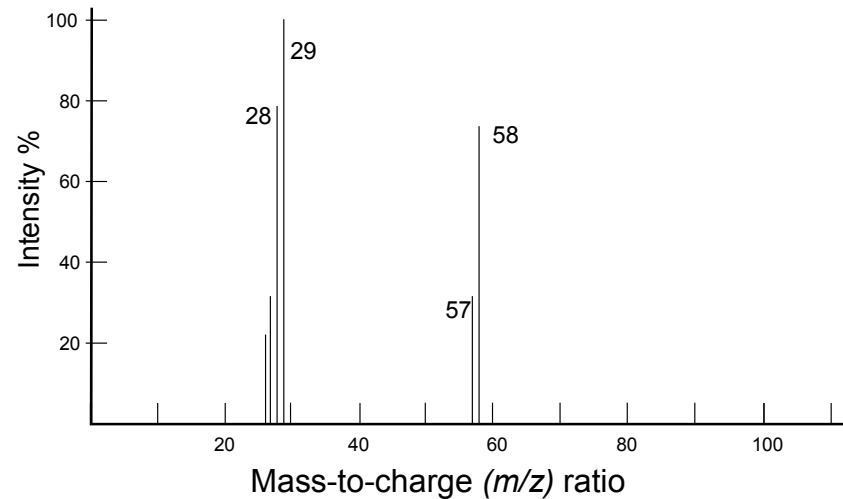
¹H magnetic resonance spectrum



¹³C magnetic resonance spectrum



Mass spectrum



Substance 38

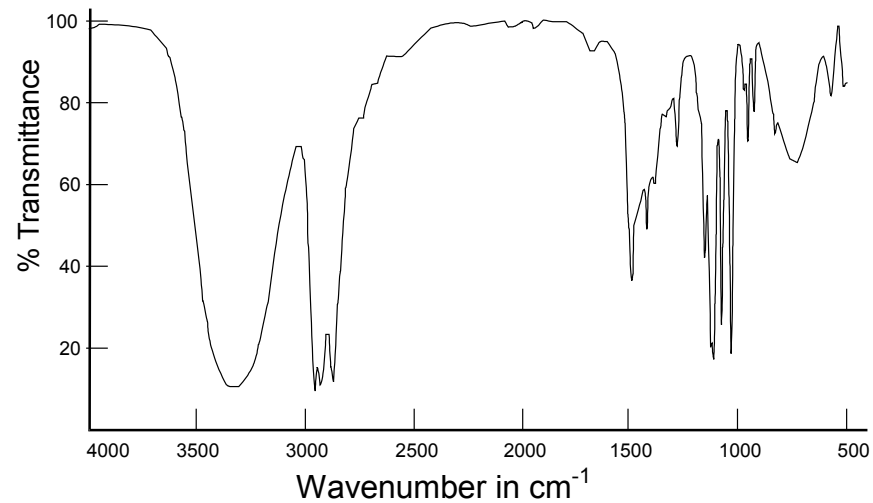
Ultra-violet spectrum

No data available

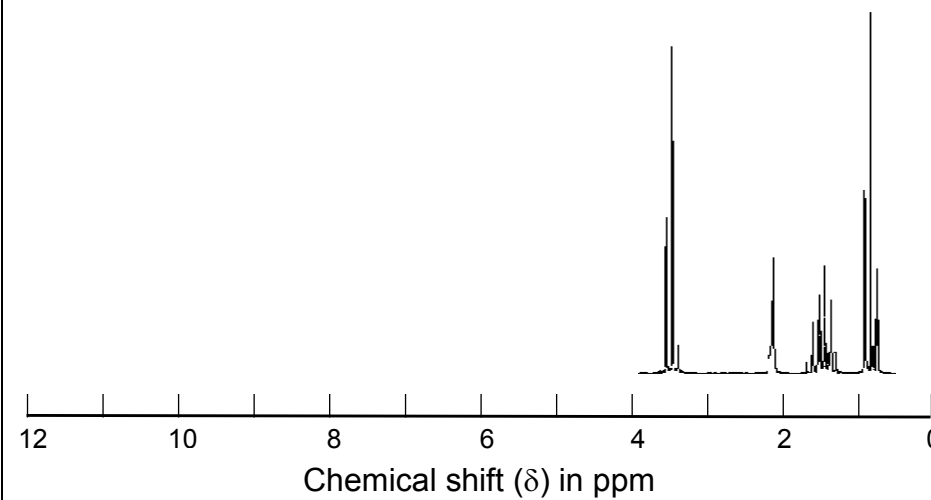
Analysis

Carbon	60.0%	Oxygen	26.7%
Hydrogen	13.4%		

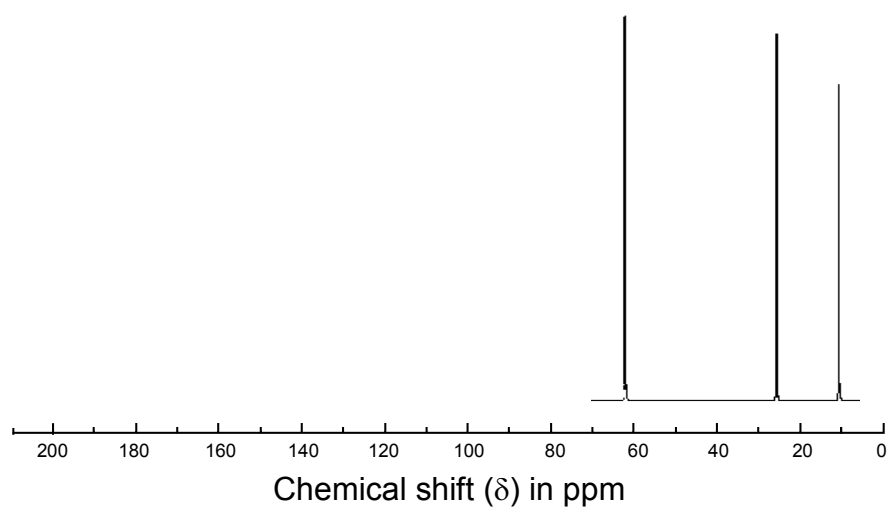
Infra-red spectrum



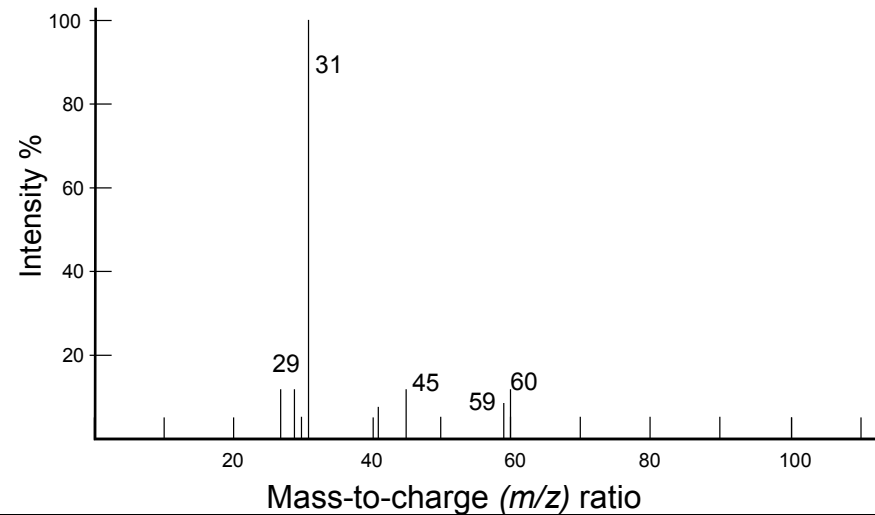
¹H magnetic resonance spectrum



¹³C magnetic resonance spectrum



Mass spectrum



Substance 39

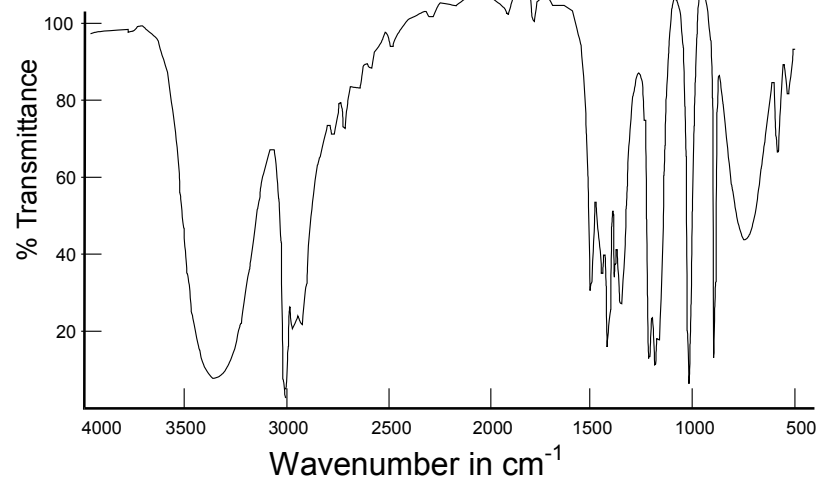
Ultra-violet spectrum

No data available

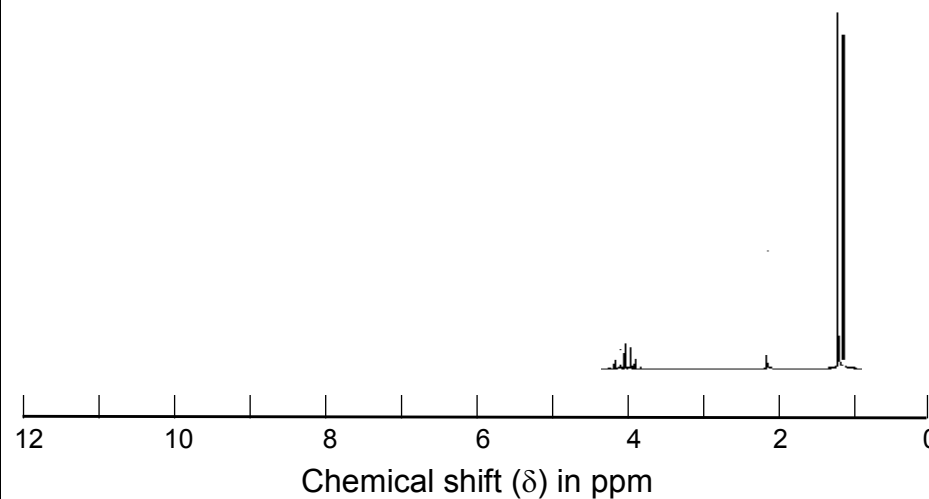
Analysis

Carbon	60.0%	Oxygen	26.7%
Hydrogen	13.4%		

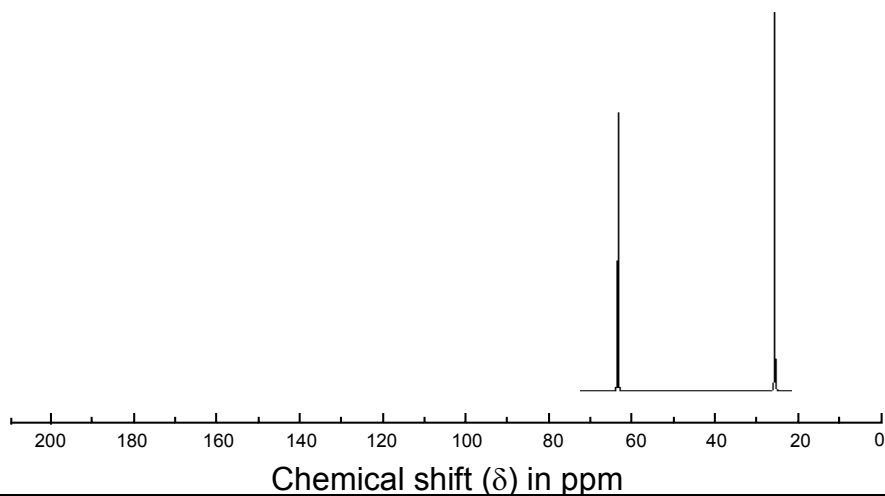
Infra-red spectrum



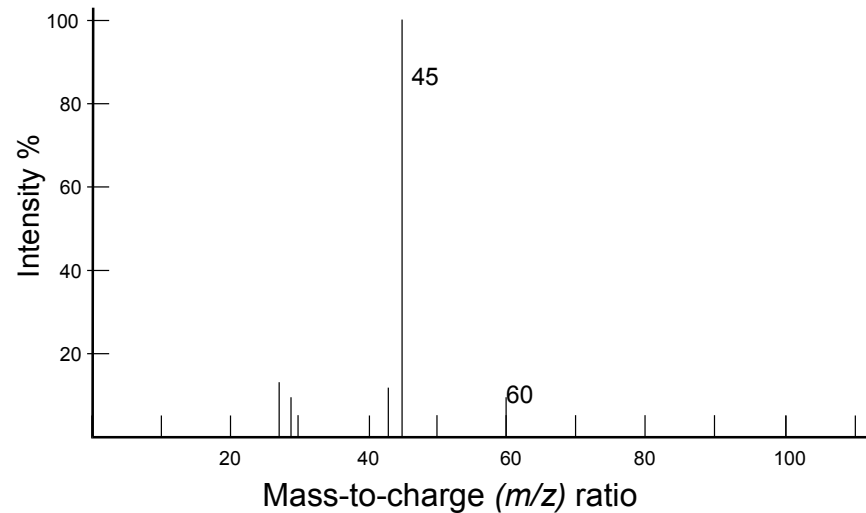
¹H magnetic resonance spectrum



¹³C magnetic resonance spectrum



Mass spectrum



Substance 40

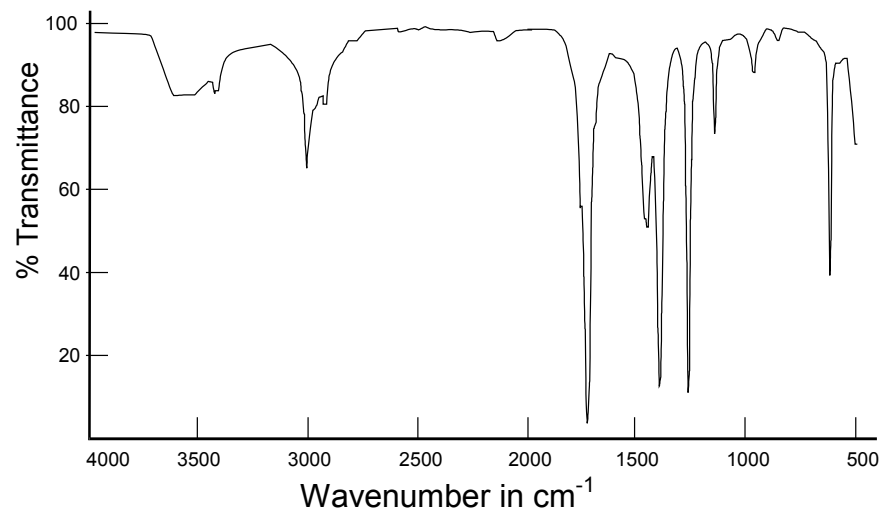
Ultra-violet spectrum

No data available

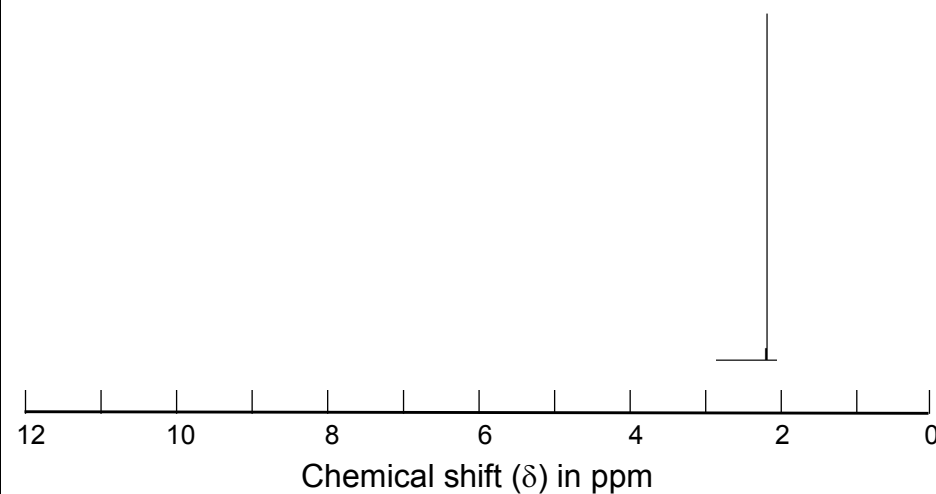
Analysis

Carbon	62.1%	Oxygen	27.6%
Hydrogen	10.3%		

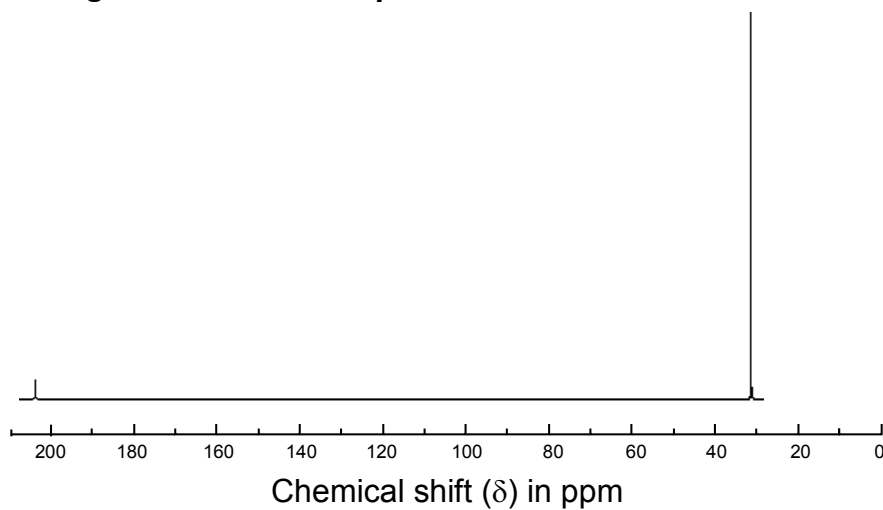
Infra-red spectrum



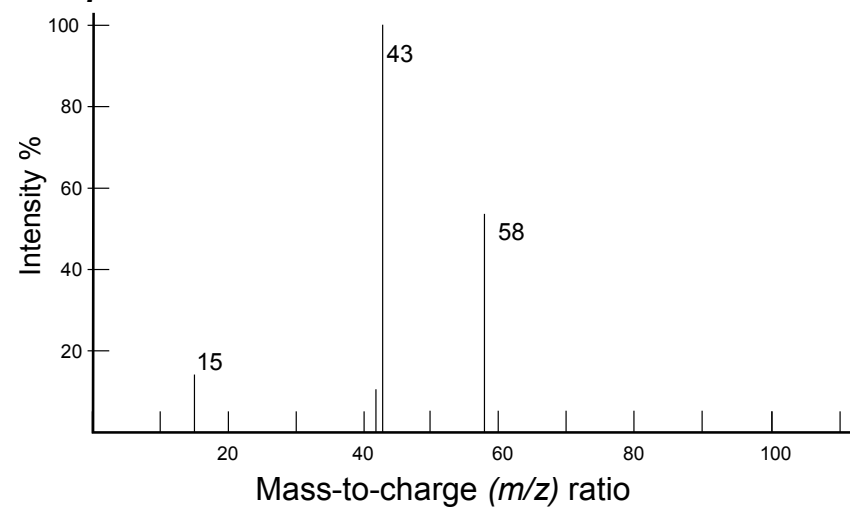
¹H magnetic resonance spectrum



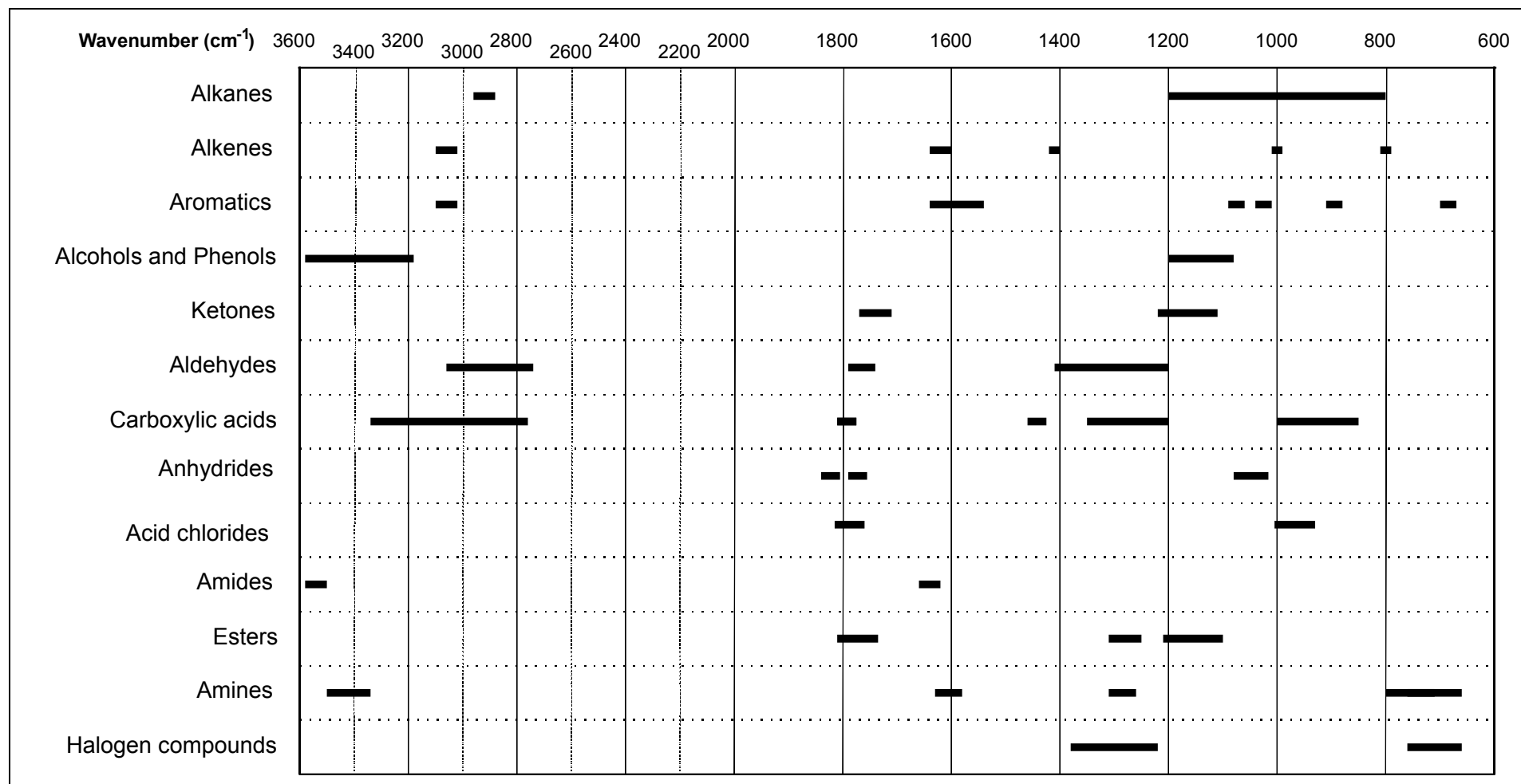
¹³C magnetic resonance spectrum



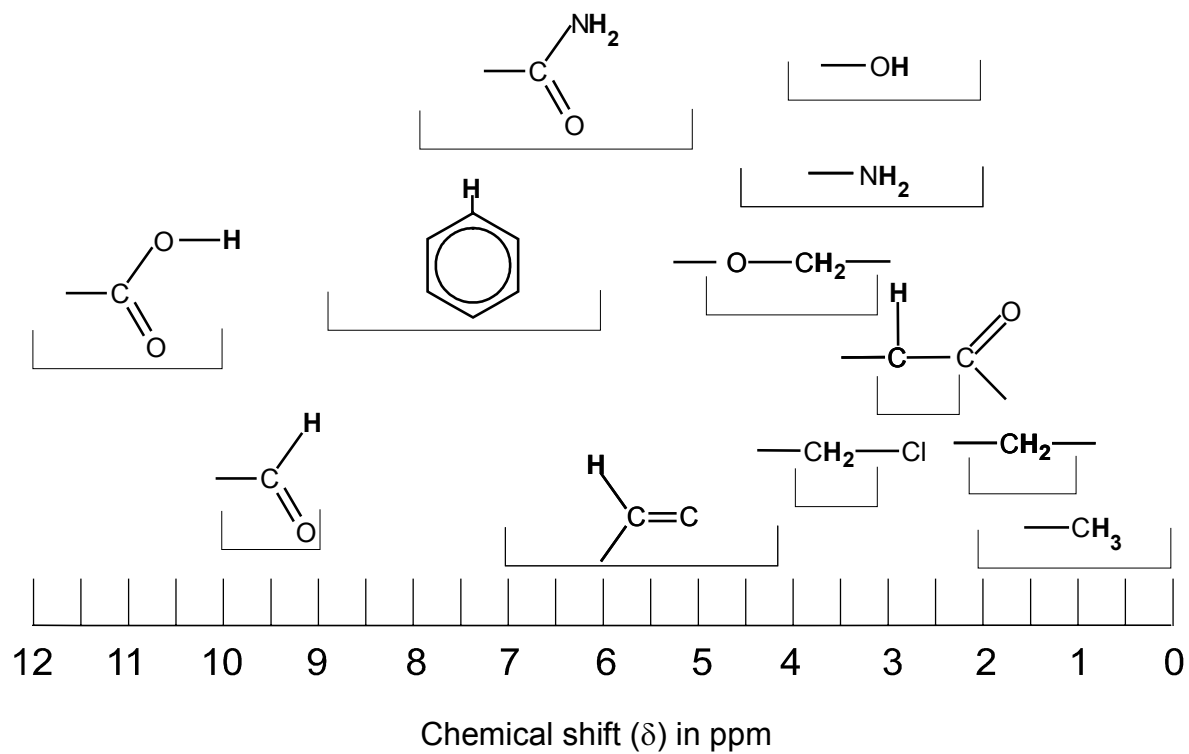
Mass spectrum



Appendix 1 Infra-red spectra correlation chart



Appendix 2 ^1H magnetic resonance spectra correlation chart



Appendix 3 ^{13}C magnetic resonance spectra correlation chart

