Infrared Spectroscopy

Question: Can we determine which label belongs to which container?

In our experiment, we are going to try to identify the substances present in a series of containers.

Aims & Objectives:

Our aim is to find out which substance is which in a series of containers that have had their labels fall off. We have a list of potential compounds that have been in stock in the past.

We will:

1) Record an IR spectrum for all the unknown substances (each student should record two, making sure to allocate substances so that each one has its spectrum recorded by at least one person in the group).
2) Predict the IR absorptions we expect to see for the candidate substances.
3) By comparing predictions with the spectra observed, try our best to narrow down the possibilities. It is possible we will have to refer to NMR spectra (recorded by our technicians in advance) to finalise the selection.

Learning Outcomes:

From this experiment you will learn how to:

1) Use an infrared spectrometer to record an IR spectrum for solids or liquids.
2) Interpret IR spectra to identify functional groups present in a compound.
3) Use IR spectroscopy alongside other spectroscopic tools to identify compounds.

Equipment:

- IR spectrometer connected to laptop and printer (provided)
- Pens, pencil
- Rule
- Print-out of this workbook (or copy the table into your school exercise book)

Method:

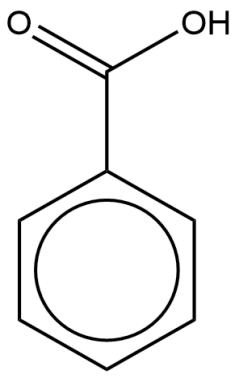
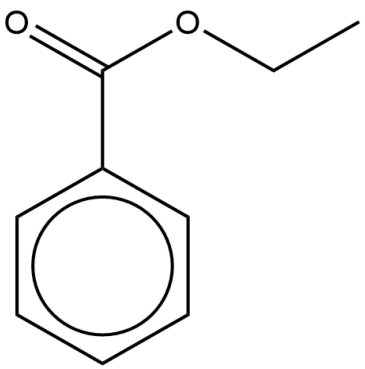
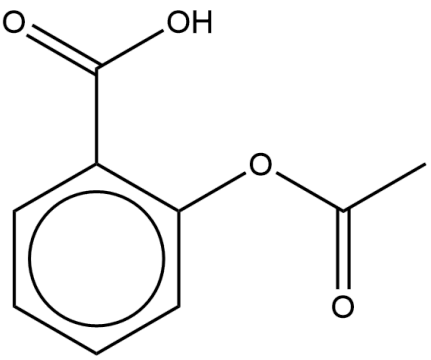
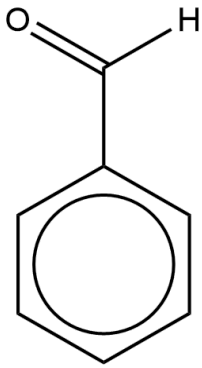
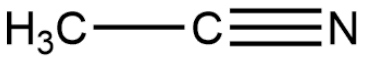
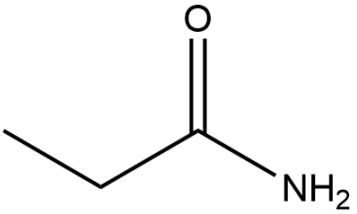
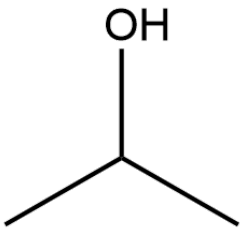
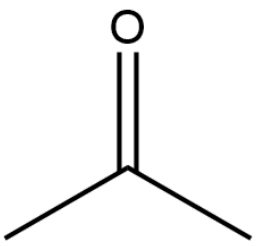
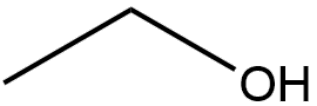
1) Watch your demonstrator illustrate how to use the spectrometer.
2) One-by-one, you will go up to collect the spectra for the two compounds you have been allocated. Make sure to get a print-out of the spectrum and clearly label which unknown substance it corresponds to.
3) When you are not using the instrument, use the table of typical stretching frequencies to make predictions about what you might expect to see in the various spectra.
4) If you are familiar with NMR spectroscopy, you can also start making predictions about the forms of the NMR spectra of the various compounds. If you are not familiar, start working through the introduction to NMR spectroscopy question on Isaac, which will hopefully familiarise you with the technique.

Experimental Data:

Make sure to collaborate with the rest of your team to identify the key absorptions seen in all the compounds, and fill out the table below accordingly.

Compound	Key absorptions
A	
B	
C	
D	
E	
F	
G	
H	
I	

Compounds

Benzoic acid 	Ethyl Benzoate 	Acetyl salicylic acid 
Benzaldehyde 	Acetonitrile 	Propionamide 
Propan-2-ol 	Propanone 	Ethanol 

Discussion:

When trying to confidently allocate compounds using IR spectroscopy, we will need reliable differences of what we expect to see in the spectra. It can be helpful to sketch a decision tree diagram that will narrow down the options based on the presence/absence of certain key peaks. Try to draw such a decision tree below.

Conclusion (we will discuss this in more detail later today):

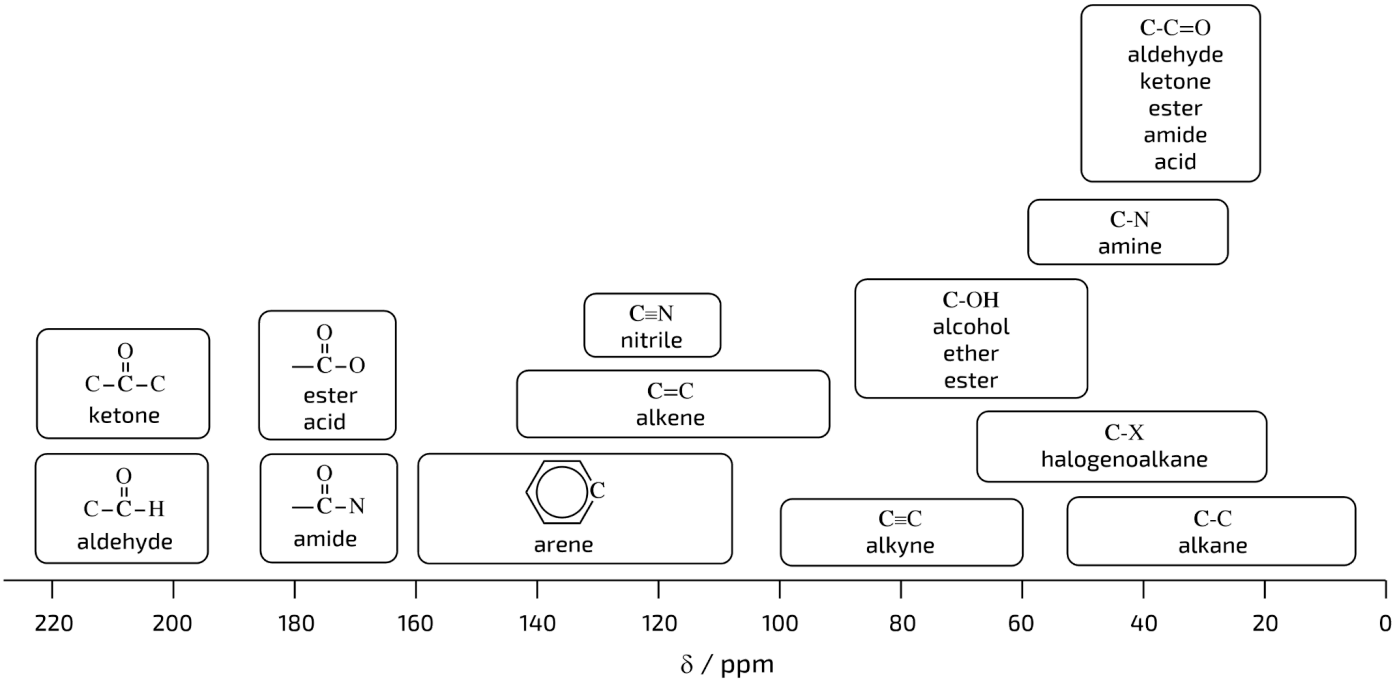
If you are confident in any of the allocations, please complete the table below. If you are unsure about some allocations, make sure to indicate the possibilities for each unknown compound, and we will finalise the allocation by using the NMR data in the theoretical session later in the day.

Compound	Allocation
A	
B	
C	
D	
E	
F	
G	
H	
I	

Characteristic infrared absorptions in organic molecules

Bond	Location	Wavenumber / cm^{-1}
C-H	Alkane	2962-2853
	Alkene	3095-3010
	Alkyne	3300
	Arene	3030
	Aldehyde	2900-2820 and 2775-2700
N-H	Amine	3500-3300
	Amide	3500-3140
O-H	Alcohols and phenols	3750-3200
	Carboxylic acids	3300-2500
C=C	Alkene	1669-1645
	Arene	1600, 1580, 1500, 1450
C=O	Aldehydes	1740-1720
	Ketones, alkyl	1720-1700
	Ketones, aryl	1700-1680
	Carboxylic acids, alkyl	1725-1700
	Carboxylic acids, aryl	1700-1680
	Carboxylic anhydrides	1850-1800 and 1790-1740
	Acyl chlorides	1795
	Acyl bromides	1810
	Esters	1750-1735
	Amides	1700-1630
C≡C	Alkynes	2260-2100
C≡N	Nitriles	2260-2215

^{13}C NMR chemical shifts relative to tetramethylsilane (TMS)



^{1}H NMR chemical shifts relative to tetramethylsilane (TMS)