

LAB 1 -2223155

by Libbie Bush

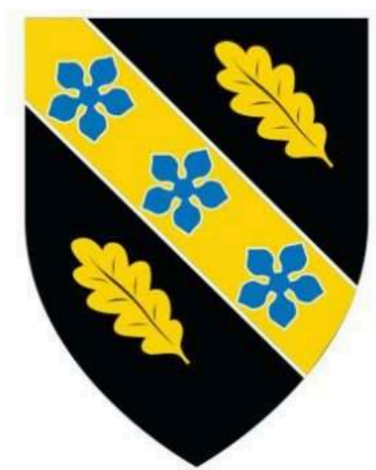
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LAB: FT-IR ANALYSIS and IDENTIFICATION OF ORGANIC MATERIALS

L6 -Advanced Chemistry of OME (ACDA6020)

2223155

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Aim

The aim of this report is to interpret the FT-IR spectra for 4 unidentified compositions. Using data collected identify the functional groups in the spectra to identify out of a list of 4 what the sample is based of its functional groups *and write detailed SOP for the FT-IR measurement.*

Hypothesis

Each of the potential 4 samples have a unique spectrum depending on the functional groups that it contains. The spectra should be a least 95% match to previous samples in the library assuming that the compassion contains some impurities.

Variables:

Independent: The samples

Dependant: The FT-IR spectrum position and shapes

Control: Instrumentation settings, background corrections, calibrations

Theory



FT-IR is a confirmative test used to identify unknown compositions. It works by shining an infrared light on a sample to see what wavelengths of light are absorbed and transmitted. The light that is not absorbed is then shown on a graph with its intensity. [1] Each functional group has a different fingerprint which is visible on the spectra produced to help identify the overall composition, however this only gives a general spectra so further test would be required if you wanted a more detailed breakdown of the compositions. These potential fingerprints are shown below:

Major Functional Group	Absorption Frequency Region			
O-H	3650-3590			
N-H	3500-3300	1650-1590	900-650	
=CH-H	3100-3070	1420-1410	900-880	
=C-H	3100-3000	2000-1600		
C-H	2900-2700	1440-1320		
=CH ₃	2880-2860	2970-2950	1380-1370	1470-1430
O-H	2700-2500	1320-1210	950-900	
C≡C	2140-2100			
C=O	1750-1700			
C=C	1600-1500			
C-N	1340-1250			
C-O-C	1200-1180			
-C-H	770-730			

Figure 1 - Functional group absorption Frequency

FT-IR has been used in EOD (explosive ordnance disposal) to help identify the type of explosives found.

Portable devices can be used to help during clean-up operations so the operators have a better

understanding of the material they have come across and can act accordingly to ensure safety. [2]



Chemicals and equipment

Chemicals

In the experiment samples A, B, C and D are unknown compositions. However, it has potential to be one of the following 4:

- Guanidine

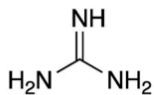


Figure 2 - Guanidine Structure [3]

- Acetaminophen

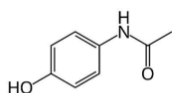


Figure 3 - Acetaminophen structure [4]

- Ascorbic acid

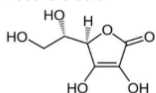


Figure 4 -ascorbic acid structure [5]

- Methyl 3 nitrobenzoate

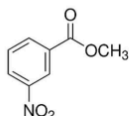


Figure 5 - Methyl 3-nitrobenzoate Structure [6]

The only hazard associated with this composition as that ascorbic acid is an oxidizer.

During this experiment an IPA is also used for cleaning purposes

Equipment

The PPE requirement for this lab is nitrile gloves and safety glasses.

A spatula is used for moving the sample to the sample plate on the machine as well as blue roll for cleaning purpose.



Figure 6 - spatulas

The FT-IR used was Perkin Elmer Spectrum two shown bellow



Figure 7 - Spectra 2 [1]

The software connected to the machine that is being used is "Spectrum IR". During the scans it has a range of $4000\text{--}450\text{ cm}^{-1}$. When a sample is being analysed it runs 15 scans then takes an average as its outputs that average in a graphical format, it does 15 scans as it is proven to be a statistically significant amount to give an accurate representation of the sample.

Procedure

1. Turn the computer and the machine on and load up the spectrum IR software
2. Take some IPA and blue cloth to wipe down the arm, foot and sample area to ensure no residue left over from any previous test
3. A background scan must be run to ensure that there is no residue left on the plate before looking at the first sample. The arm is pulled towards the sample area till it is over it and then the foot is twisted till you have hear the ratchet click.
4. On monitor with the software open click the background scan and let it run till a graph is displayed.
5. The following graph must be displayed before continuing

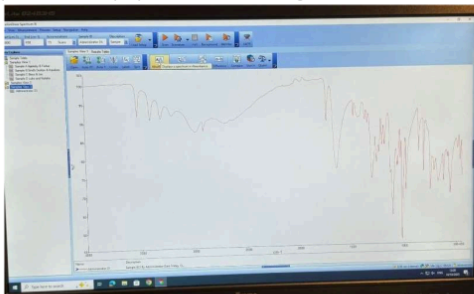


Figure 8 - background scan

If it does not repeat the previous steps. This shows the machine is set up and clean before use.
This background is subtracted from the results so will not impact the spectra

6. Twist the foot to raise it and push the arm away from the sample area. Using a spatula take a rice sized portion and place it on the sample area. Example is shown below:

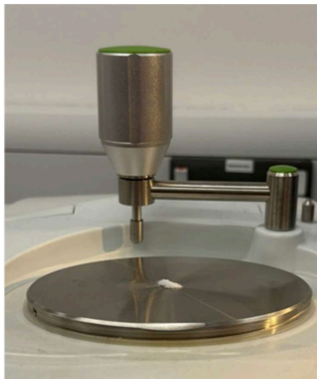


Figure 9 - sample in place

7. Make sure it is all covered then bring the arm back over the sample area and twist the foot back down until it clicks.
8. Select scan on the software, it will run a preview scan then a full analysis which will show you the full spectra
9. The spectra are then compared to others that are in the library for the system to help determine composition the material. If the sample has a 95% similarity, then it can be accepted as that composition.
10. Save the file locally to the pc naming the samples A, B, C or D with the date of completion
11. Repeat the steps 1-4 to ensure the sample plate and foot are clean, any waste will be placed in the general waste bins. Once these are complete then move on to the next sample until all samples are complete

Results and Discussion:

Sample A

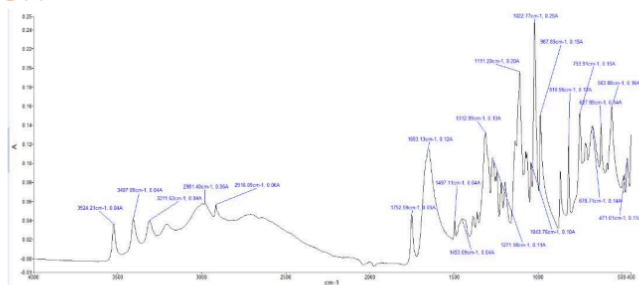


Figure 10 - sample A graph

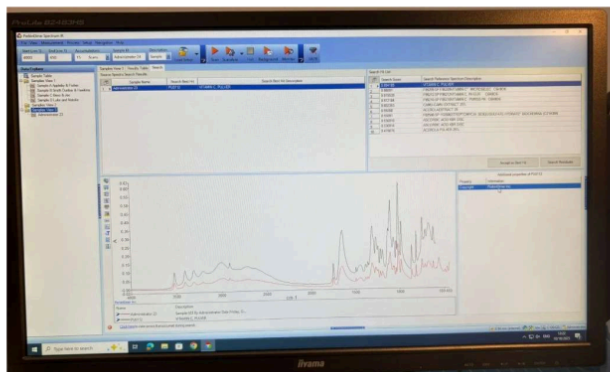


Figure 11 - sample A comparison

Sample A has a 99% similarity to vitamin C powder which is another name for Ascorbic acid, there for sample a is Ascorbic acid

Sample B

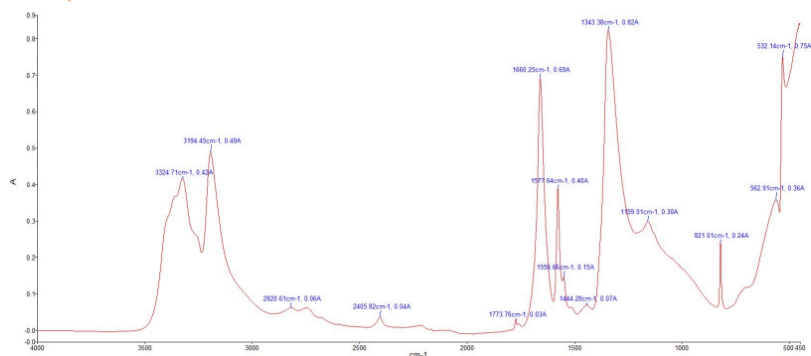


Figure 12 - sample B graph

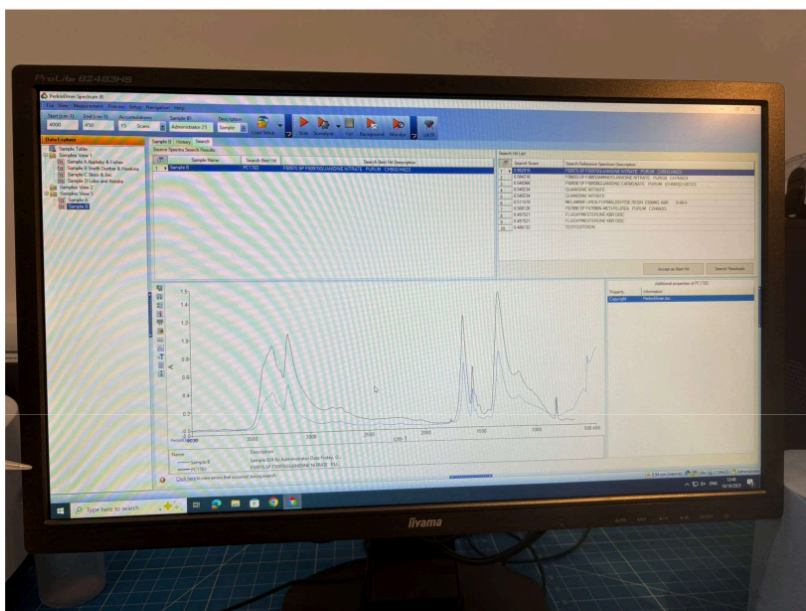


Figure 13 - sample B comparison

Sample B has a 95% similarity to s Guanidine there for sample B is Guanidine

Sample C

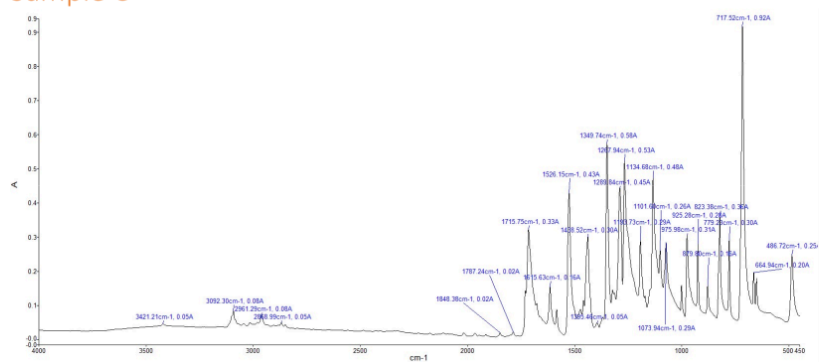


Figure 14 - sample C graph

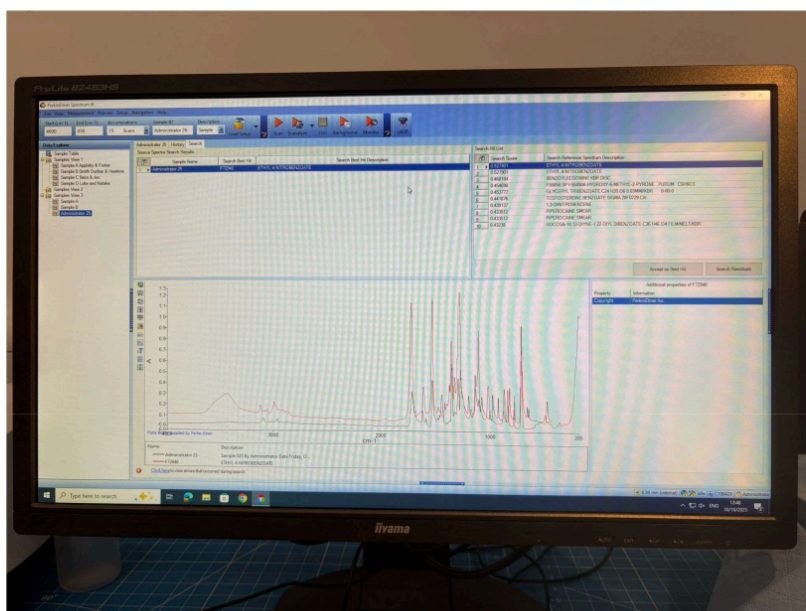


Figure 15 - sample C comparison

Sample c has a 55% similarity to ethyl 4-nitrobenzoate, this is not any one of the expected 4 samples however looking at the graph and there peaks its looks like Methyl 3-nitrobenzoate, this is also found in ethyl 4-nitrobenzoate. We can conclude that sample C is likely to be Methyl 3-nitrobenzoate

Sample D

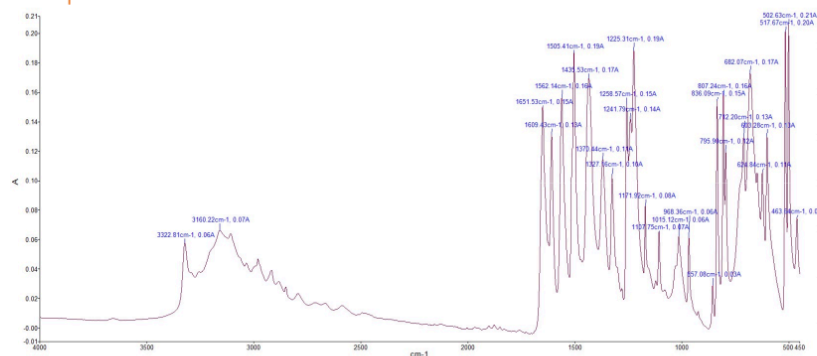


Figure 16 - Sample D Graph

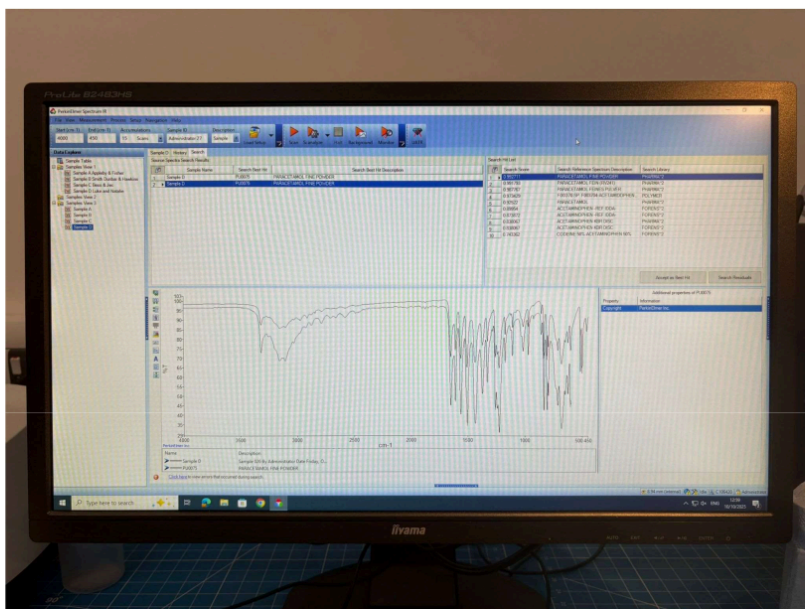


Figure 17 - sample D comparison

Sample D has 99% similarity to parastomal which is another name for acetaminophen therefore sample D is Aceptaminophen

Conclusions

Overall, this experiment is a goof way of showcasing how FT-IR can help identify compounds however contamination can make a huge different to the spectra and potentially lead to a miss- identification of the compositions, it also relies on the same set up every time of constant results which can be hard to achieve.

References

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Engagement with Literature 10/15

You use several online sources, but the range is limited and many references are basic websites rather than high-quality technical or academic FT-IR literature. Several spectral claims (e.g., O-H, N-H, C=O assignments) are not directly supported by cited ranges. The literature engagement is acceptable but not sufficiently strong for Level 6.

Knowledge and Understanding 11/20

You show a basic understanding of FT-IR and functional groups, and your sample identifications are correct. However, the introduction frames the task using a hypothesis and variables, which are only one part of the report. Professional SOP is not mentioned. Essential theory is missing: vibrational modes (stretching, bending, rocking, twisting) are not described, and ATR physics is barely addressed. Functional-group identification on spectra would add clarity, but this was not used consistently.

Cognitive and Intellectual Skills 12/20

Interpretation is mostly descriptive. You correctly identify each sample, but peak assignments are brief and not justified with literature. The fingerprint region is not analysed, and there is little discussion of peak shape, intensity, or why peaks may shift (e.g., ATR effects, hydrogen bonding). Comparison to reference spectra is used, but the reasoning needs more depth and selectivity.

Practical Skills 8/30

This is the weakest section. The method is not reproducible and lacks nearly all essential FT-IR parameters required for an SOP-level procedure.

Transferable Skills 11/15

The report is neatly formatted with clear figures and logical structure. Writing is readable, though sometimes informal. Figures are included but peak labels are minimal. Hypothesis/variables section reduces professional tone. Presentation is generally adequate.

PAGE 1

PAGE 2

PAGE 3

Text Comment. and write detailed SOP for the FT-IR measurement.

**Comment 1**

it can also be used to determine the purity of known samples

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PAGE 4



Comment 3

good point

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