

FTIR Lab

by Natalie Coplin

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Advanced Chemistry of OME - ACDA6020

Laboratory Report – Fourier Transform Infrared Analysis of Organic Compounds

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1. Introduction

The purpose of this experiment is to confirm key functional groups of four unlabelled samples, each corresponding to one of the following: guanidine, acetaminophen, ascorbic acid and methyl 3-nitrobenzoate. Each of these compounds are often used in the design, manufacture or disposal of energetic compounds. Confirmation of their identity will enable safe disposal by preventing incorrect mixing of chemicals and reducing the risk of any unplanned reactions. Analysis will be performed using Attenuated Total Reflectance - Fourier Transform Infrared Spectroscopy (ATR-FTIR) and obtaining spectra for each of the samples.

1.1. Hypothesis

Four samples have been provided: guanidine, acetaminophen, ascorbic acid and methyl 3-nitrobenzoate. By determining and comparing the specific functional groups of each compound, each Fourier Transform Infrared Spectroscopy (FTIR) spectra will correspond to one of these samples.

1.2. Predicted Outcome

The samples are expected to exhibit distinct functional groups on each spectrum, enabling identification.

Figure 1, shows the structure of guanidine. It is expected to display bands for -NH_2 (amino) and C=N groups.

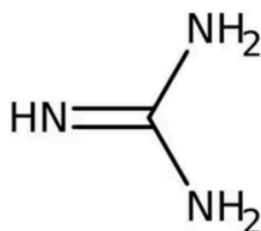


Figure 1 Chemical structure of Guanidine [1]

Acetaminophen is expected to exhibit a band for a phenol group (-OH), an aromatic ring and an amide group with both C=O carbonyl group and a N-H bond, these groups can be seen in Figure 2.

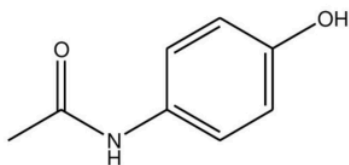


Figure 2 Acetaminophen structure [2]

Ascorbic acid, shown in Figure 3, is expected to exhibit a broad O-H stretching band due to four hydroxyl groups, and a C=O band characteristic of a lactone ring.

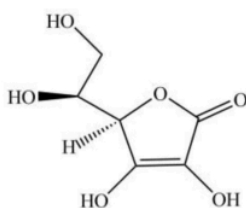


Figure 3 Structure of ascorbic acid [3]

Methyl 3-nitrobenzoate is expected to exhibit an ester group (-COOCH₃) and a nitro-group (NO₂) attached to an aromatic ring, as shown in Figure 4.

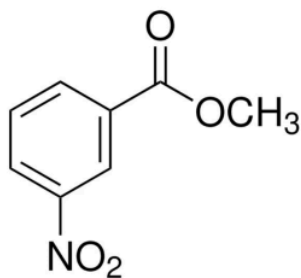


Figure 4 Chemical structure of methyl 3-nitrobenzoate [4]

1.3. Key Variables

For this experiment the variables are:

Independent – samples under test

Dependent – resulting ATR-FTIR spectra

Control – crystal type, instrument settings, cleaning method, sample contact pressure.

1.4. FTIR

FTIR is a widely used largely non-destructive method for the identification of compounds based on the vibrations of functional groups when light is passed through the sample. The frequency at which a sample absorbs radiation and the intensity of the absorption is measured to produce a spectrum [5]. To do this, infrared radiation of a known wavelength range is directed at the sample through a beam splitter. The light is reflected by two mirrors, one of which is fixed while the other can move. The reflected light recombines at the beam splitter and it then directed to the sample. Some of which will transmit through, while some is absorbed [6]. The transmitted light is measured and a Fourier Transform applied to convert raw data into a readable spectrum of either transmittance or absorbance [7] [8]. The vibrations of the functional groups vary depending upon the bonds in the compound, with each bond absorbing a different amount of energy and producing a corresponding peak on the spectrum.

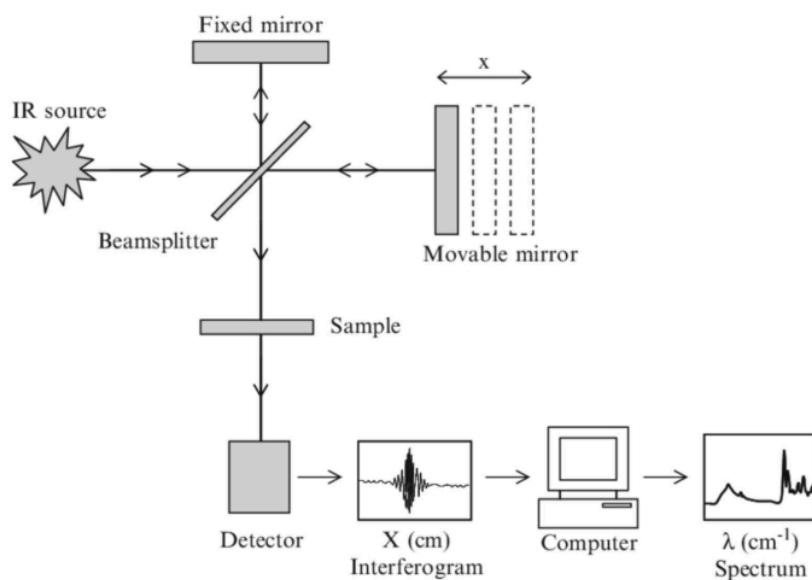


Figure 5 FTIR spectrometer features [9]

ATR-FTIR relies on total internal reflection of the beam, with the crystal having a higher refractive index than the sample. When the beam strikes the internal surface of the crystal, at an angle above the critical angle, it undergoes total internal reflection, producing an evanescent wave which interacts with only the first few microns of the sample. Due to this, sample preparation is minimal. [10], [11].

1.5. Importance of FTIR in Energetics

FTIR is commonly used in laboratories and in the field for the identification of explosive compounds [12]. In field tests allow samples to be analysed without the need for transportation and the potential increase in risk of an unplanned reaction or explosion. As FTIR is non-destructive, it is valuable where there is limited quantity of sample available for test. FTIR can be used in manufacture and through-life monitoring of samples, due to the formation or loss of functional groups. Additionally, it can detect contamination in samples, revealing impurities which may impact the stability or reactivity of a compound [13]. This helps ensure the expected stability, performance and reliability can be maintained.

2. Methodology

2.1. Equipment and Personal Protective Equipment (PPE)

- Samples for analysis.
- FTIR spectrometer and computer.
- Laboratory coat.
- Safety glasses.
- Nitrile gloves.
- Blue roll.
- Isopropyl alcohol.
- Bin for waste disposal.

2.2. Procedure

1. Before starting the experiment put on the required PPE. This experiment is considered low risk; however, standard laboratory PPE should be worn.

Ensure the computer and Perkin Elmer Spectrum Two FTIR spectrometer are switched on, with the Spectrum IR software running. If either of these are not ready to use, seek assistance from the technician. The spectrometer will be in the configuration shown in Figure 6. Background scans will have already been run therefore there is no need for the student to conduct these.



Figure 6 FTIR Spectrometer

2. Select the correct anvil for the type of sample, referring to Figure 7 for guidance. These are located at the back right on the machine behind the arm. Attach the anvil onto the base of the arm, as shown in Figure 8, by firmly pushing.

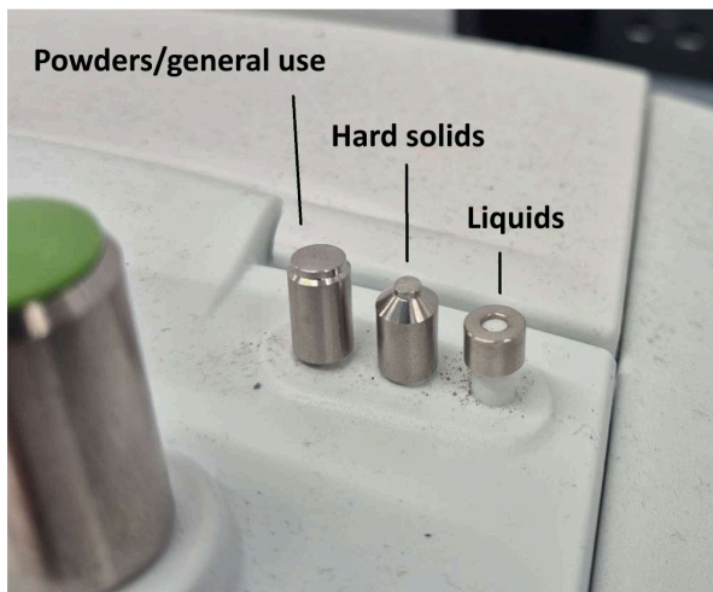


Figure 7 Anvil options

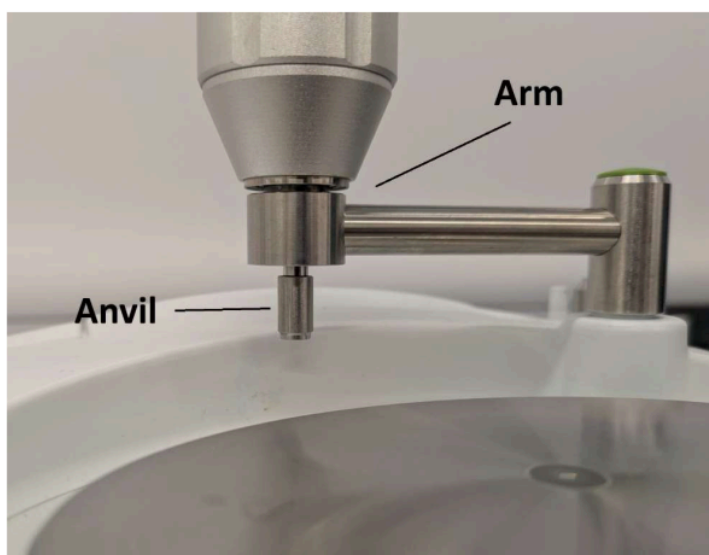


Figure 8 Anvil fitted to arm

3. With a lint free tissue and isopropyl alcohol, clean the plate, crystal and anvil. Dry with a clean tissue.

4. Using a spatula place enough sample on the crystal to completely cover it. The crystal is shown in Figure 9.

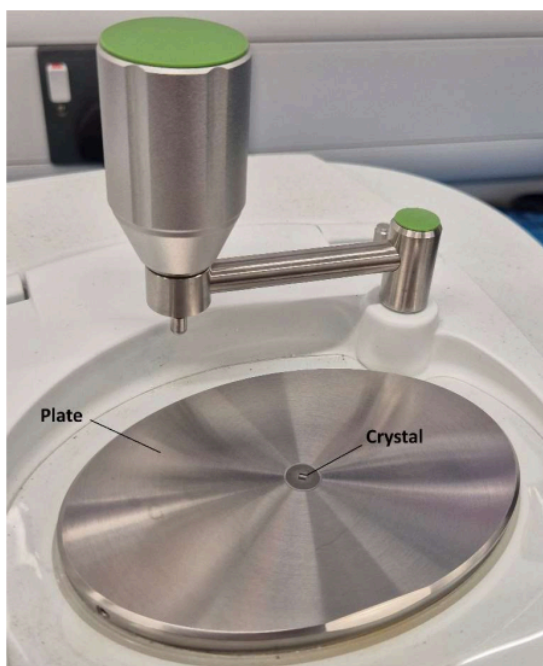


Figure 9 Plate and crystal

5. Rotate the arm anticlockwise until it is over the sample. Turn the green knob clockwise until the ratchet clicks over at the preset tension, indicating sufficient pressure and contact with the sample.
6. In the Spectrum Two software check the number of scans is set to 15, under 'accumulations' – shown in Figure 10.

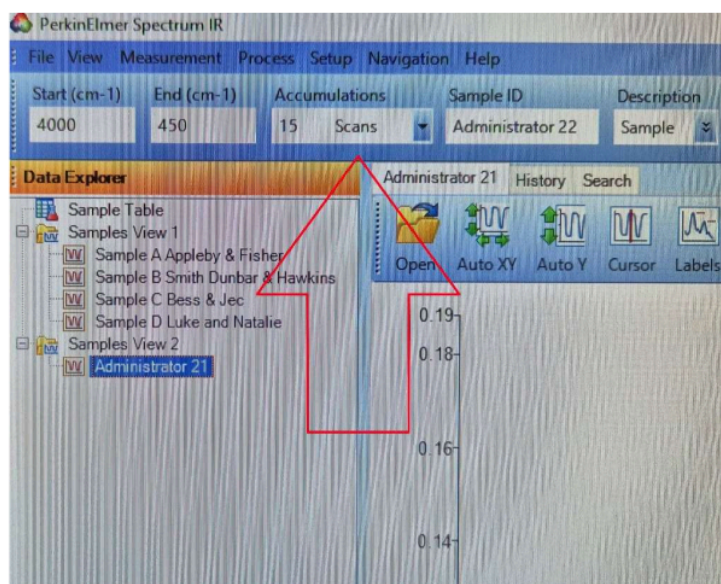


Figure 10 Number of sample scans (accumulations)

7. Click 'preview scan'. This provides a quick overview of the sample showing if it is clean and useable. If the preview returns a poor spectrum, refer to Appendix 1 for guidance.
8. With an acceptable preview scan, click 'scan' again to run a full scan. This will perform 15 individual scans in the spectral range of 4000 cm^{-1} to 450 cm^{-1} and negates the need for manual repeat tests.
9. A high-quality spectrum should be produced, if this is not the case refer to Appendix 1. The software automatically produces a transmittance spectrum; this is easily changed to absorbance by clicking 'absorbance' – highlighted in Figure 11.

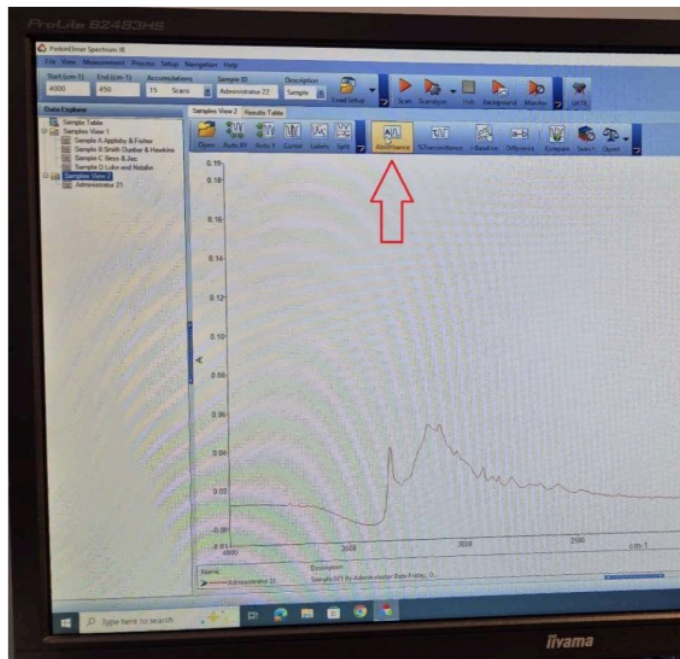


Figure 11 Absorbance spectrum button

10. Compare the spectrum to the library by clicking 'search' – shown in Figure 12. This has been configured to search all 14466 samples held in the library. A search score will be shown alongside potential material matches, indicating the confidence limit for the sample to that material. A 95% match or higher is considered acceptable.

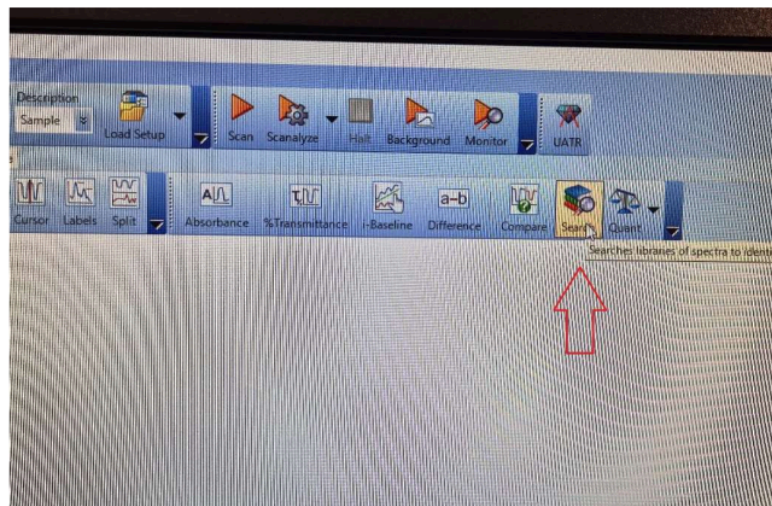


Figure 12 Search function in software

Search results and search score (percentage match) are shown in Figure 12.

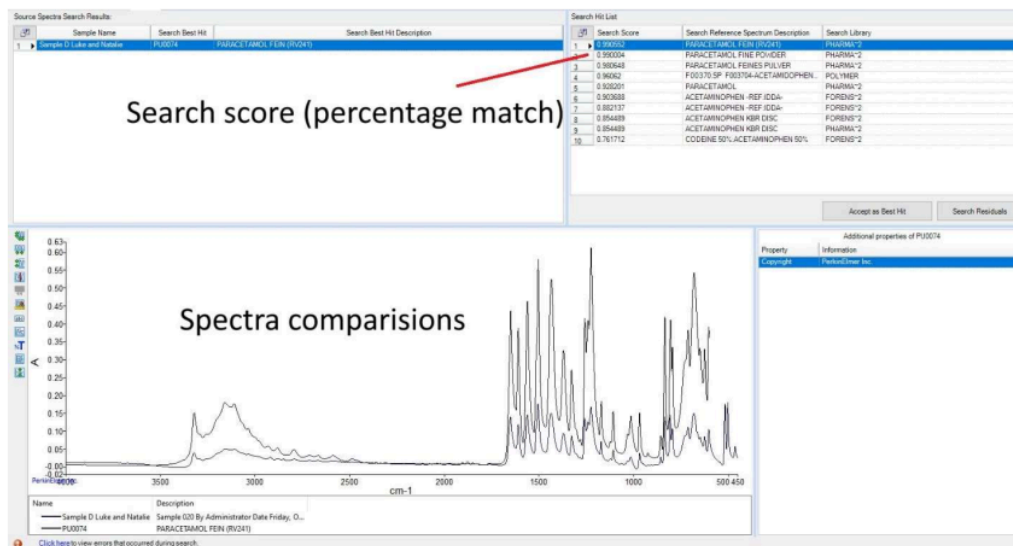


Figure 13 Library search results for acetaminophen

- When finished with the sample, twist the green knob on the arm anti-clockwise to lift the foot. Rotate the green arm clockwise to expose the crystal. Clean the plate, foot and crystal with IPA and lint free tissue, ensuring all waste is disposed of through appropriate routes. The FTIR and computer can be left running. Remove the anvil and place back on the holder, cover the crystal with the arm (or alternative cover if provided).

A quick reference guide for the Perkin Elmer Spectrum II can be found in Appendix 1.

3. Results

Figure 14 to Figure 17 show the spectra obtained from the scans for each of the four samples with each peak wave number labelled.

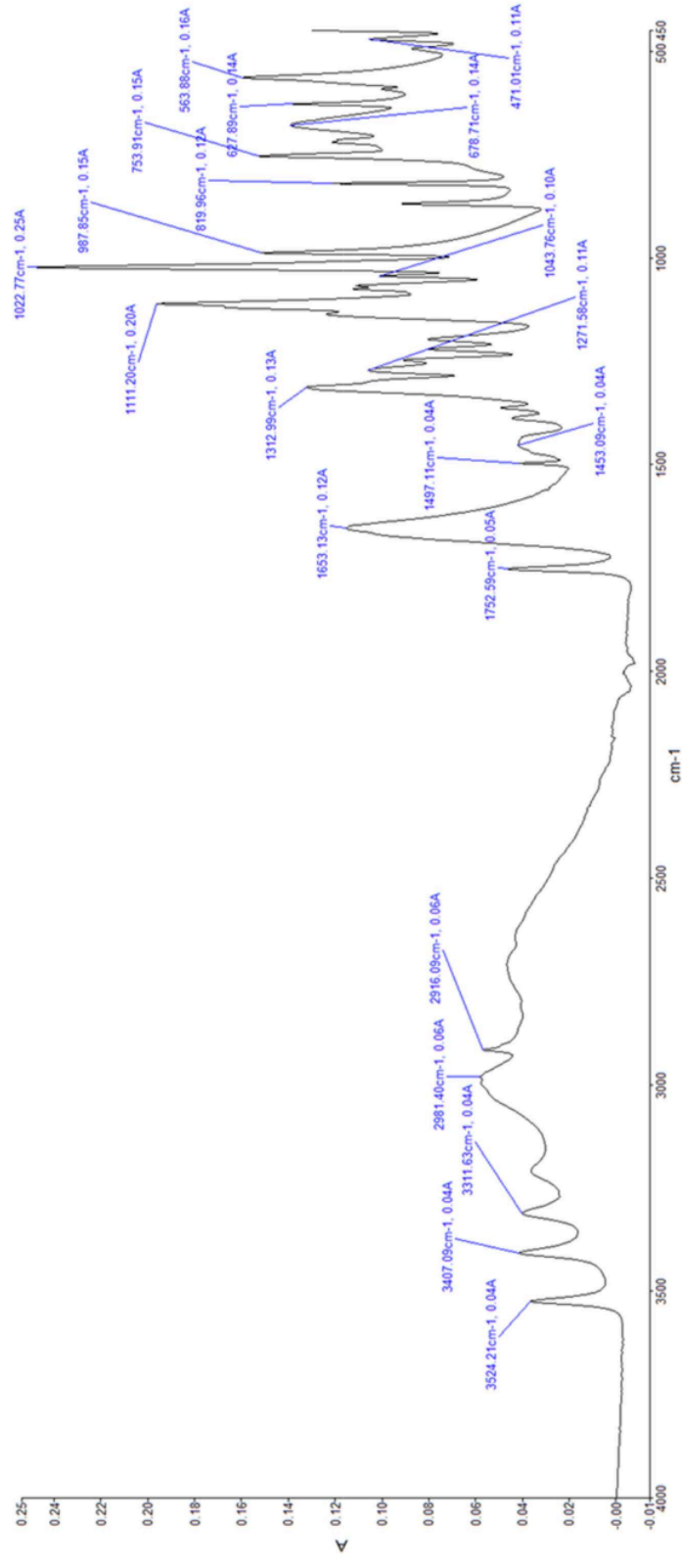


Figure 14 FTIR spectrum for sample A

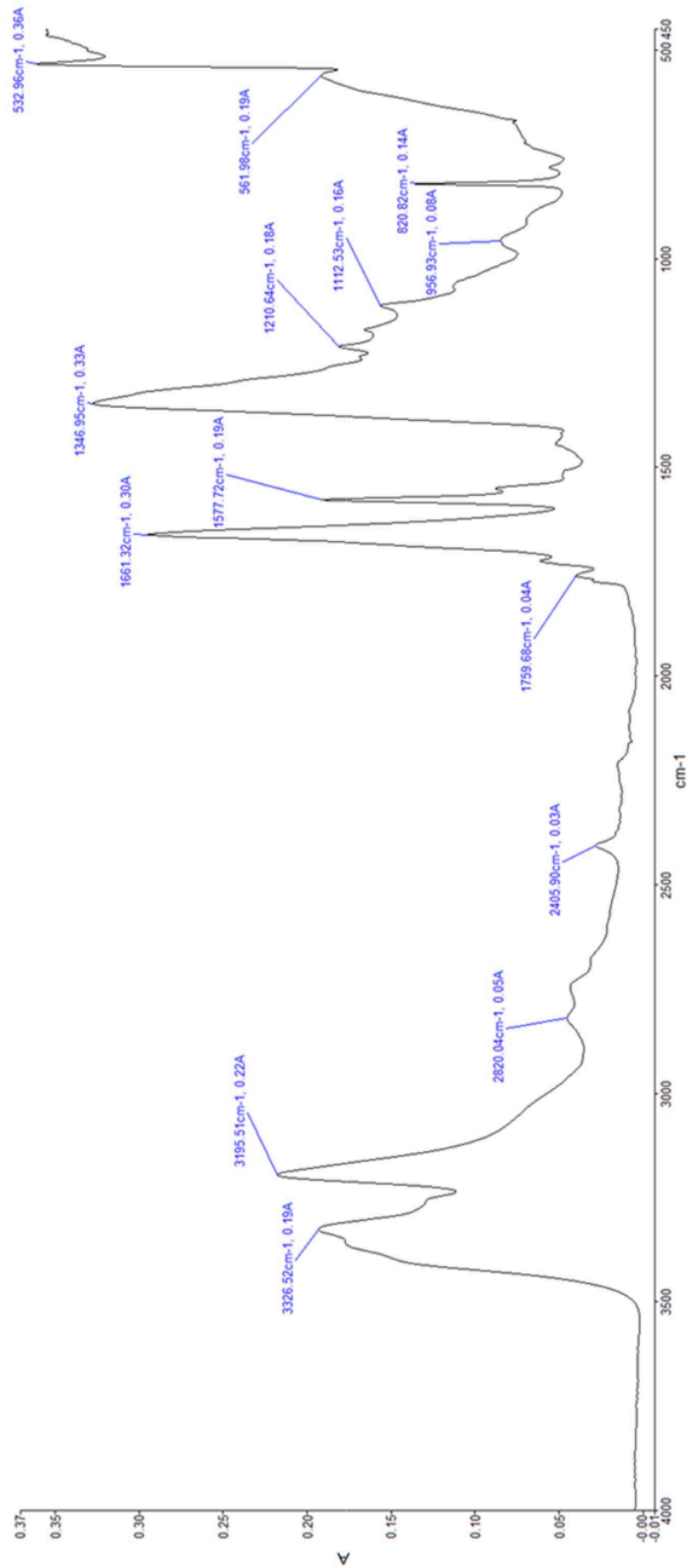


Figure 15 FTIR spectrum for sample B

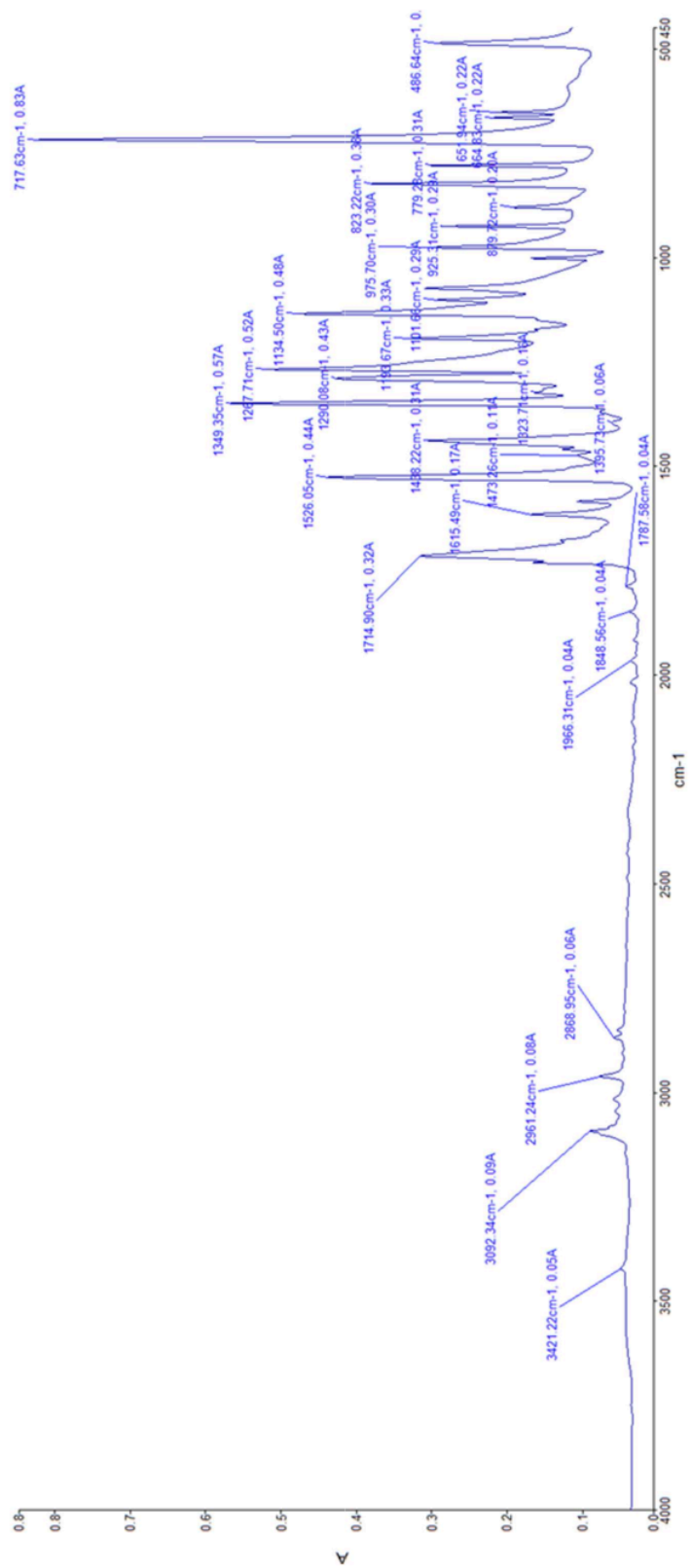


Figure 16 FTIR spectrum for sample C

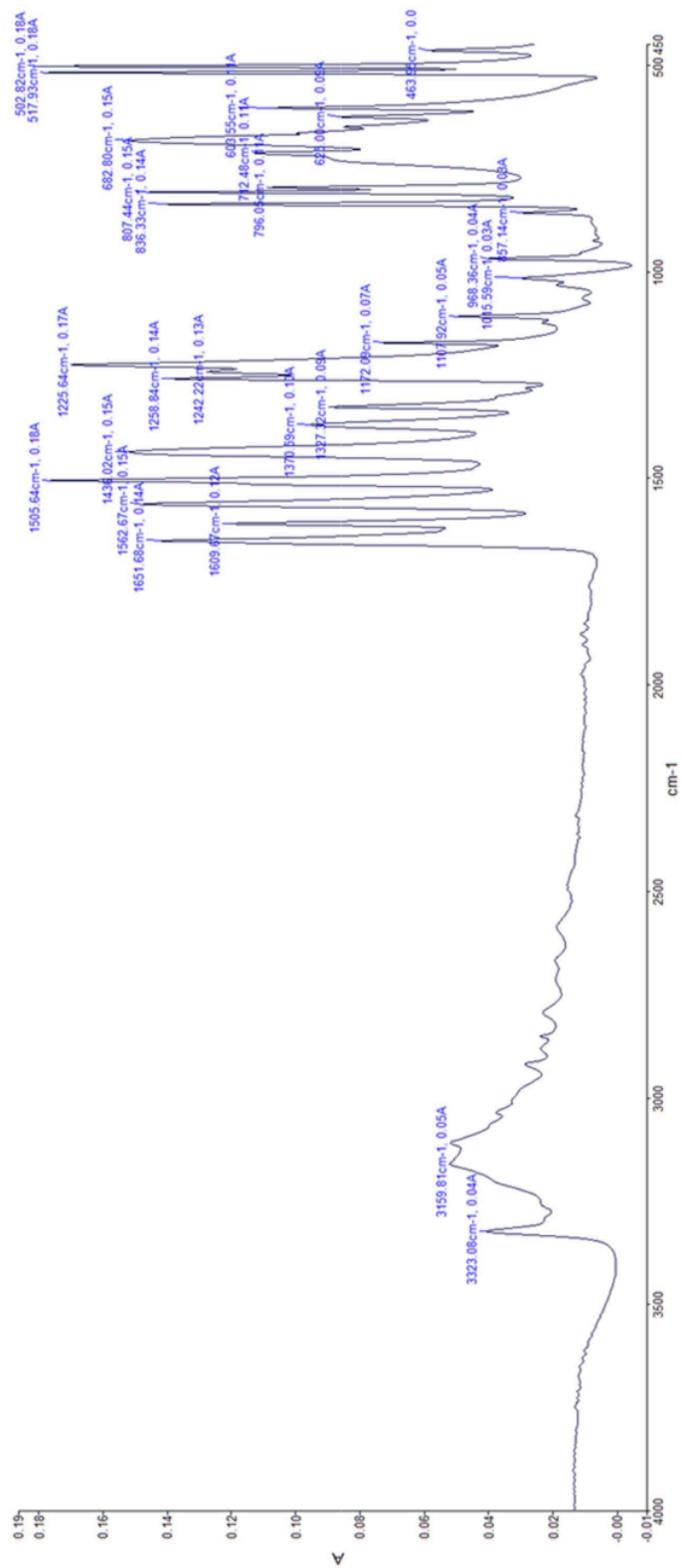


Figure 17 FTIR spectrum for sample D

4. Observations

Using information provided in the brief and literature, key general and fingerprint peaks were identified in each spectrum from the four compounds analysed [14], [15], [16], [17], [18], [19], [20] [21]. This information is summarised in Table 1 showing the peak and the wave number – noting that overlap and shifting of peaks may have introduced some error.

Table 1 Key peaks identified from FTIR spectra

Sample ID	Key general peaks/function groups	Wave number (cm ⁻¹)	Key fingerprint peaks/functional groups	Wave number (cm ⁻¹)
A - ascorbic acid	O-H broad stretch (hydroxyl)	3524, 3311	C-O stretch (lactone)	1022-1312
	C-H stretch	2916, 2981	O-H bend	987
	C=O stretch (lactone)	1752	C-H bend	753
B - guanidine	N-H stretch	3326, 3195	C-N	1346
	C=N stretch	1661		
C - methyl 3 benzoate	N-O asymmetric stretch (nitro)	1526	N-O symmetric stretch	1349
	C=O (ester)	1714	C-H bend (aromatic)	717
D - acetaminophen	N-H stretch	3323	C-N stretch (amide)	1258
	O-H broad (phenol)	3159	C-H bend (aromatic)	807, 836
	C=O stretch	1609		
	N-H bend	1562		

By identifying key peaks in both the general and the fingerprint region [22], it was possible to determine which spectra likely corresponded to each sample. For example, methyl 3-nitrobenzoate is the only compound in the tests to contain N-O bonds, while ascorbic acid is the only compound that features a lactone ring. Guanidine and acetaminophen both contain N-H bonds; however, guanidine lacks a benzene ring whereas acetaminophen contains one. The peaks noted in Table 1 support the predicted outcomes from *1.2 Predicted Outcome*.

By way of confirmation the library search results have been included in Appendix 2. The percentage match from the library search is as follows:

- Ascorbic acid – 99.4%
- Guanidine – 99.5% (to guanidine nitrate)
- Methyl 3-nitrobenzoate – 52.6%
- Acetaminophen – 99.1%

Methyl 3-nitrobenzoate has a lower percentage match with compounds in the library than ideal. It was noted during testing the library does not contain a reference spectrum for methyl 3-nitrobenzoate, so a good match will not be possible. In this case it is possible to state this compound is likely to be methyl 3-nitrobenzoate due to a partial match from the library, identification of key functional groups from the spectrum and through a process of elimination

with the other samples, given the information in the brief states that one sample is methyl 3-nitrobenzoate.

5. Discussion

Each of the identified compounds have applications to the energetic world.

Ascorbic acid has been used as a fuel substitute in black powder mixtures. It acts as a reducing agent, reacting with potassium nitrate to produce gas and heat, burning cleaner than conventional black powder [23][24].

Guanidine (nitrate) is an explosive precursor that can be nitrated into nitroguanidine using sulphuric acid [25], [26]. It is used extensively in the energetic field from triple-base gun propellants to shock insensitive high explosives [27].

Cranfield University has been studying the use of acetaminophen as an inert substitute for High Melting Explosive (HMX), due to similar crystal properties [28]. This approach helps to establish good research methods before applying the techniques to energetic materials.

Methyl 3-nitrobenzoate is used in the manufacture of explosives. Since the compound is a nitro aromatic, it can be used as a precursor to a more energetic material [29] [30].

6. Conclusion

By examining FTIR spectra it was possible to determine the four unlabelled compounds, which was confirmed through comparison of a spectral library search. Sample A was identified as ascorbic acid, sample B as guanidine, sample C as methyl 3-nitrobenzoate and sample D as acetaminophen.

These results highlight the effectiveness of FTIR in identifying unknown compounds, by determination of key functional groups. The minimal sample preparation and rapid analysis is particularly valuable in the detection of explosive compounds both in the laboratory and in the field.

Future work could consider validation of the samples through a complementary technique such as Raman spectroscopy or gas chromatography - mass spectrometry which would provide additional structural information. This would provide additional confidence in any results obtained.

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8. Appendix 1

Table 2 provides an overview of some common problems associated with ATR-FTIR and how they might be resolved. In each case, seek guidance from the technician where further clarity or assistance is needed.

Table 2 ATR-FTIR Troubleshooting Guide

Problem	Cause	Solution
Additional peaks	Sample contamination from residues during collection, moisture or contact with other materials	Obtain another sample where possible. If possible clean the sample and remove contamination - seek guidance from the technician.
Additional or wavy peaks, weak signal	Improper cleaning	Properly clean and dry the crystal, plate and anvil, ensures no residue, samples or fibre remains. Re-run the sample.
Weak signal intensity	Inconsistent or incorrect pressure on the sample from the arm causing limited penetration of light into the sample and/or scattering of the beam	Ensure the arm is correctly ratcheted down, turn until the first click. Re-run the sample.
Weak signal intensity or missing peaks	Crystal not covered, IR beam interacts with sample and air	Ensure crystal is fully covered with sample and ratchet is correctly applied. Re-run sample.

Table 3 provides a quick reference guide to the key parameters for the Perkin Elmer Spectrum II. These should not need to be changed. Guidance from the technician should be sought if there is a need for alternative settings or for help troubleshooting.

Table 3 Table 3 Quick reference guide to Perkin Elmer Spectrum II settings

Quick Reference Guide	
Waste route	Provided bin
FTIR spectrometer	Perkin Elmer Spectrum II
Accessory	ATR accessory
ATR crystal type	Synthetic diamond
Software	Spectrum IR
Cleaning solvent	Isopropyl alcohol
Spectral range (cm ⁻¹)	4000-450
Resolution (cm ⁻¹)	0.5
Background scans	15
Sample scans	15
File type	.csv
Baseline correction	None
Smoothing	None
Library search	Yes
Acceptance threshold (%)	95
Blank between samples	No
Replicate acquisition	Yes (automatic 15 scans)
Clean crystal between samples?	Yes

9. Appendix 2 – Library search results

Spectra from the analysed samples and library matched spectra are shown in Figure 18 to Figure 21. They show the percentage match of the library entry to that of the unknown sample, providing level of confidence (or not) in the composition of the sample.

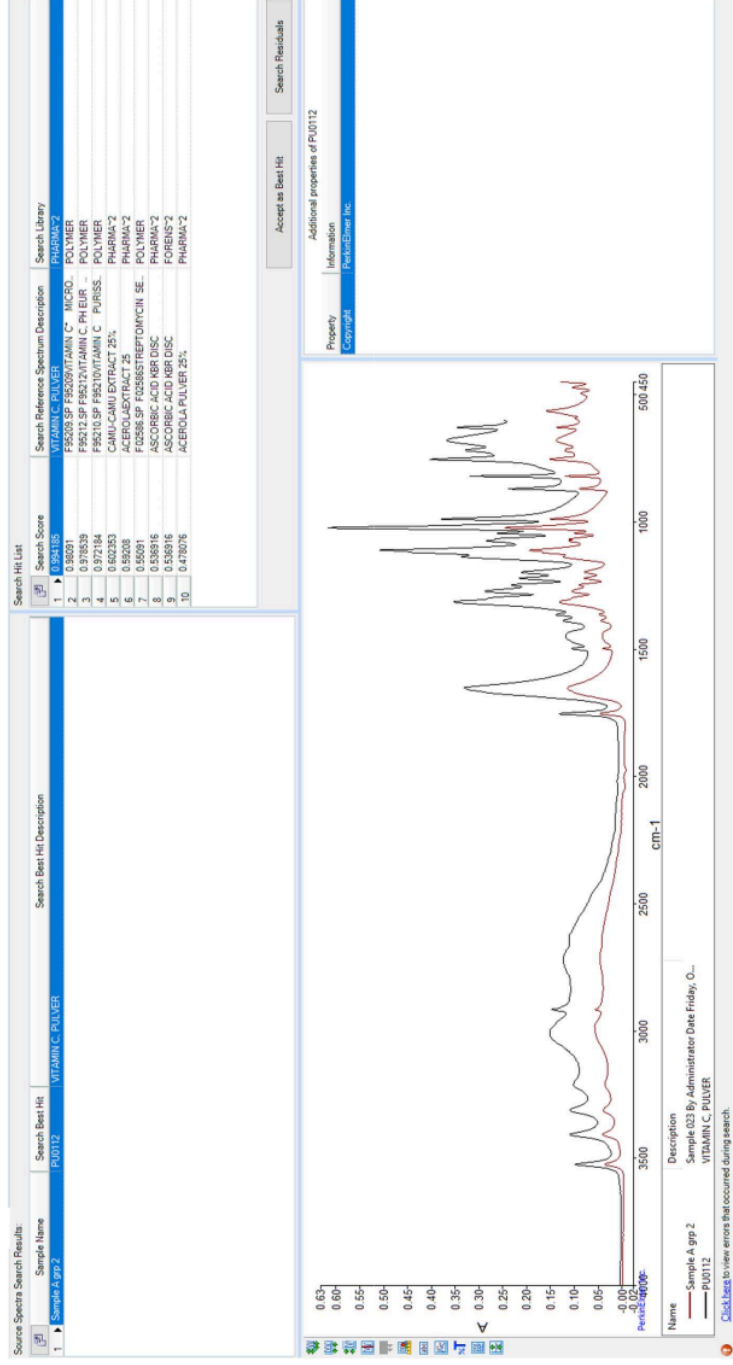


Figure 18 Sample A - ascorbic acid

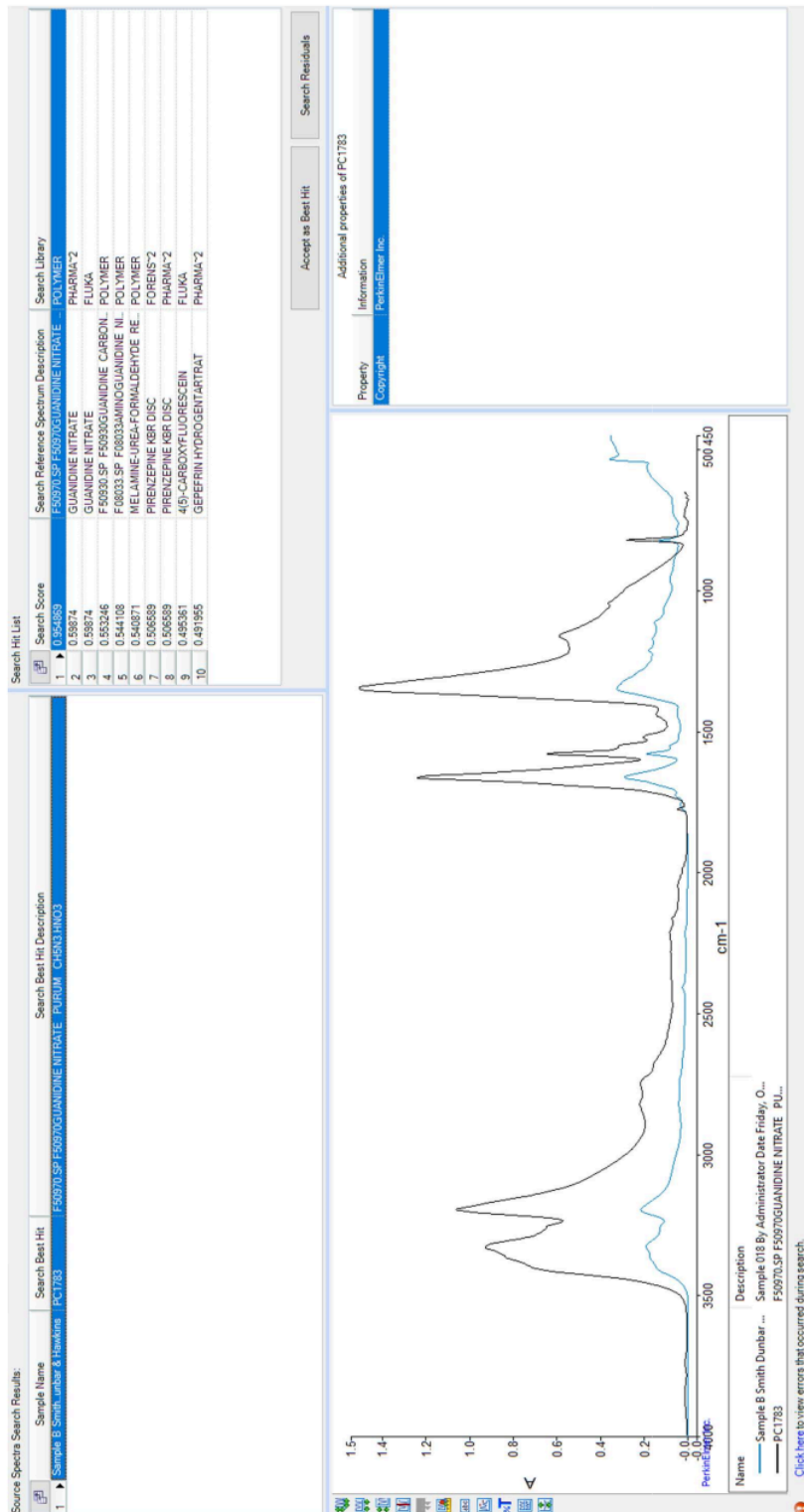


Figure 19 Sample B - guanidine nitrate

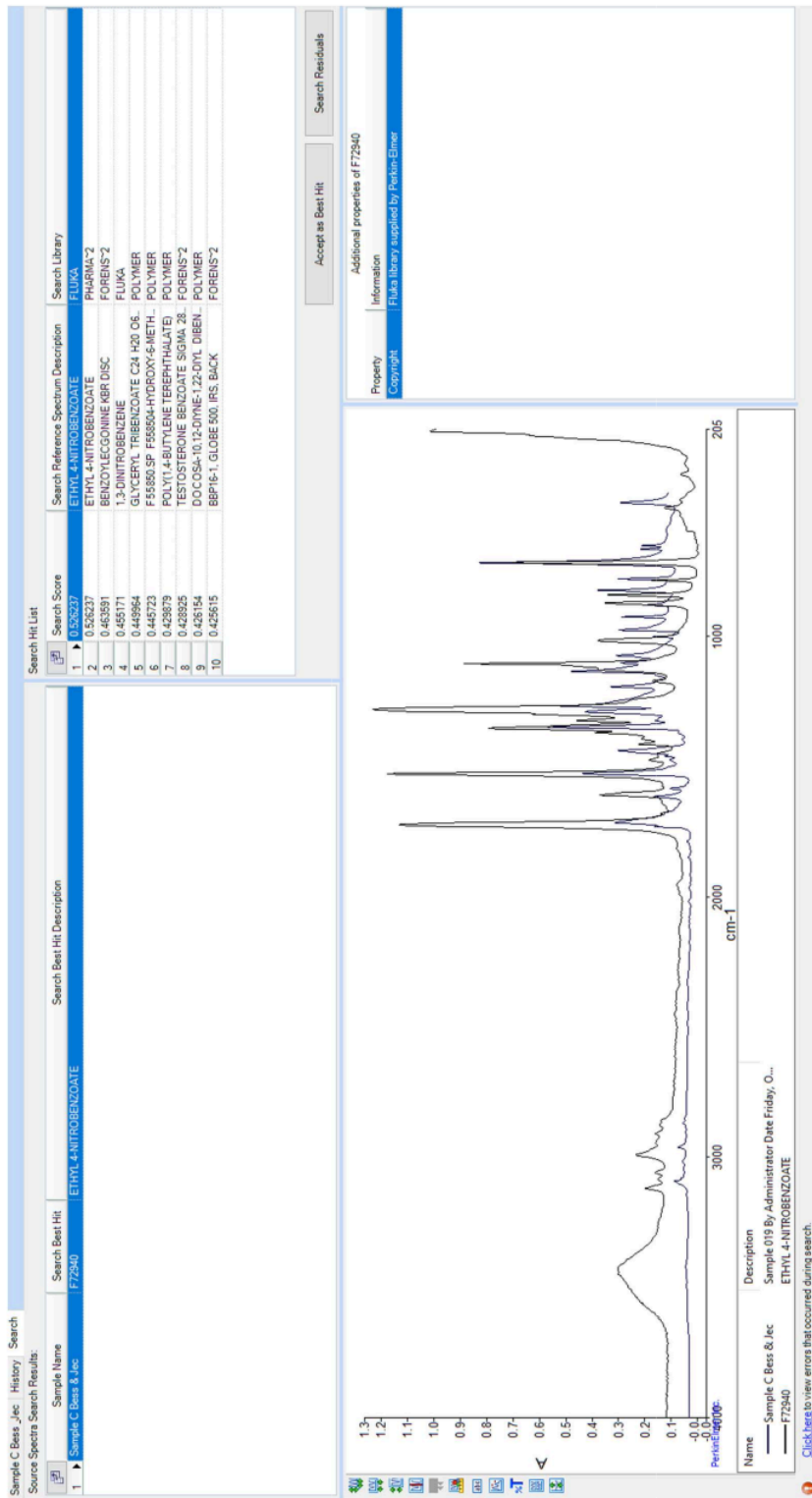


Figure 20 Methyl 3-nitrobenzoate

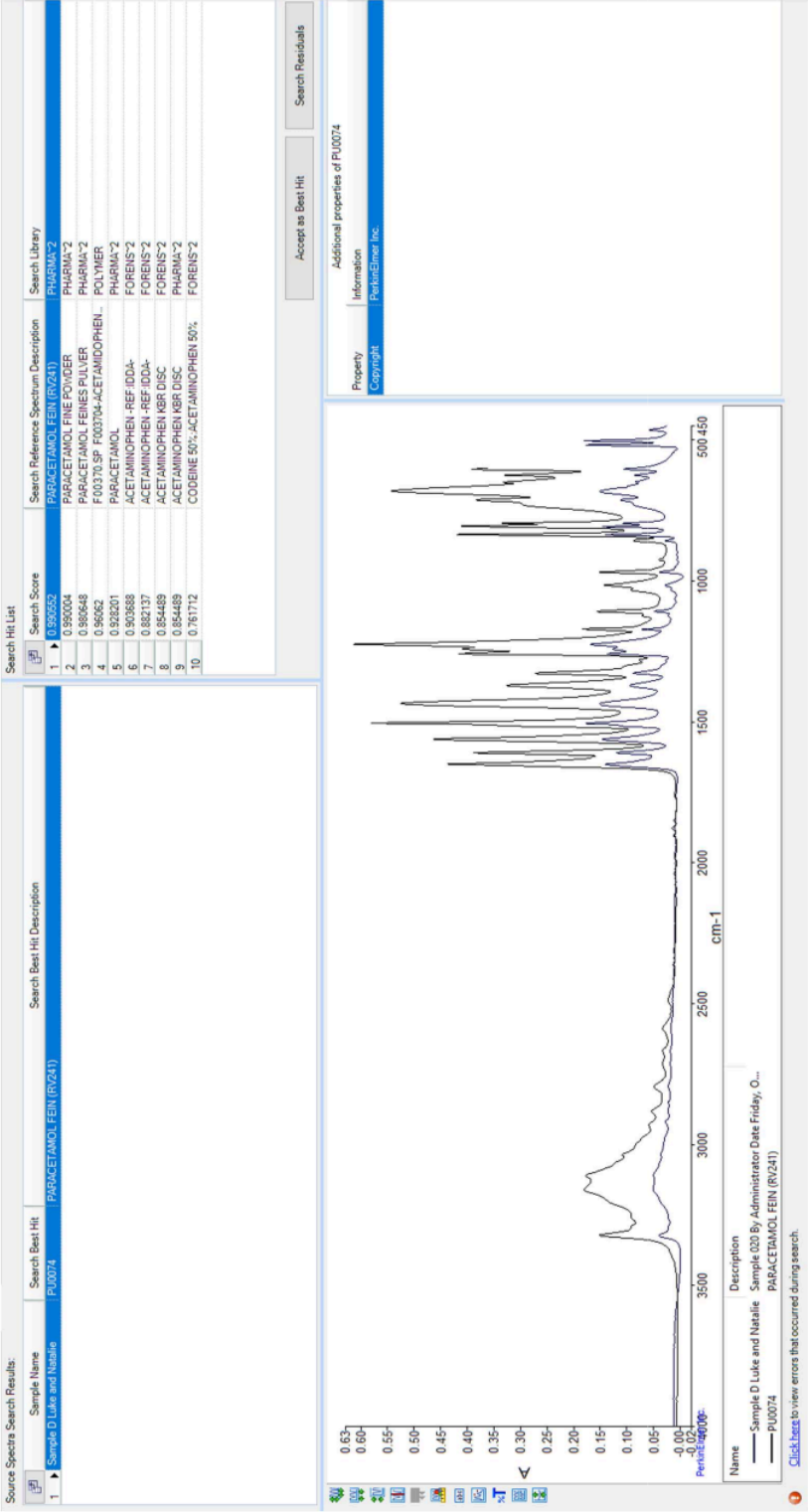


Figure 21 Acetaminophen

FINAL GRADE

73/100

GENERAL COMMENTS

Engagement with Literature 12/15

Excellent range of references including online materials and high-quality academic or technical FT-IR literature. Reference formatting is consistent, but engagement remains largely descriptive.

Knowledge and Understanding 15/20

You demonstrate good understanding of FT-IR and ATR principles, and your functional-group predictions based on structure are correct. However, the introduction incorrectly frames the work around a hypothesis and variables, and skips the SOP. Vibrational modes (stretching, bending, rocking, wagging, twisting), the basis of IR absorption, are not clearly explained. Identifying functional groups directly on the spectra would improve clarity.

Cognitive and Intellectual Skills 15/20

You identify the four unknown samples correctly and use reasonable functional-group reasoning. Structural diagrams help support your interpretation. The discussion is thoughtful and links chemical features to spectral evidence. However, fingerprint-region analysis is limited, and some reasoning is descriptive rather than analytical.

Practical Skills 18/30

relation to OME is recognised. The procedure is very clear and well structured it still lacks the SOP-level detail required by the brief. Missing parameters include: baseline and smoothing information, scan speed, QC criteria (clean background, S/N checks, re-run triggers). Without these, the method cannot be fully reproduced.

Transferable Skills 13/15

A well-presented report with excellent structure, clear diagrams and professional formatting. Writing is concise, and figures are well selected. Minor issues with overlong sections and unnecessary hypothesis framing, but overall very strong presentation.

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