

MF Lab1

by Max Fisher

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ACDA6020 LAB #1

FTIR Analysis and Identification of Organic Materials

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Introduction

This report will highlight compounds detected from 4 samples recovered from an facility researching new energetic formulation. The samples were believed to be common laboratory or industrial chemicals which require specific identification before processing and disposal. The following report will explain the methods used to identify these samples providing the likely matches.

Background

The samples provided were recovered in plastic containers and transported to the ordnance munitions an explosives lab at the University of Wales Trinity Saint David SA1 Campus.

Method

Equipment and software used:

- FT-IR spectrometer (Perkin Elmer Spectrum 2)
- FT-IR surface plate: (Perkin Elmer UATR 2)
- Desktop computer with 'Spectrum IR' Software.
- Small Plastic Weighing boat (x4)
- Metal Spatula (x1)
- Safety Googles (x1)
- Nitrile Gloves (x4)
- Isopropyl alcohol (for cleaning)
- Paper Towel (for cleaning)

Before undertaking any tasking, first gloves and safety goggles were donned.

A small sample was first decanted from its recovery container into a small plastic weighing boat; this was done using a metal spatula.

Next the FTIR instrument was prepared for use by cleaning the sample area (the spectrometer used had a diamond crystal). This was done by flushing the crystal with Isopropyl alcohol (IPA) and wiping with Paper towel, ensuring that the surface was free from contamination.

Using the computer control software, a background check was conducted to ensure than any residues remaining from the IPA would not significantly influence the results. To that extent the software was set to conduct 15 scans. It is important to conduct the same number or greater of background scans before conducting sample scans. The Spectral range set for these scans was $4000\text{-}4450\text{cm}^{-1}$

A small quantity of each sample was then placed onto the sensor, covering it completely to ensure that the material would be fully exposed to the laser.

Now that the sample was in place, the FTIR head was lowered using the ratcheting knob. It was tightened until the ratchet head clicked. This indicates the appropriate force is applied to the sample, without overstressing any components.

Using the computer 15 sample scans were then conducted again using the $4000\text{-}450\text{cm}^{-1}$ spectral range. The software averaged the results of the 15 scans to create a single graph, but no other smoothing methods were used. The use of multiple scans reduces the effect of the samples physical properties such as reflectivity on the FTIR results, enabling more accurate identification.

The file generate was compared with an inbuilt spectral database which the author of the report does not currently have access to. This provisionally identified each material. However, the following section will detail the full identification process used. The file was then saved with the following convention: SampleX_Tester_Tester.csv

Finally, the sensor was again cleaned using the IPA and the small sample disposed of in the appropriate bin.

This was repeated for each of the four recovered samples.

the method is incomplete, it doesn't include all parameters that should be set up and it is not in format of SOP

Results

Sample A

Error! Reference source not found. shows the spectra generated for sample A. The peaks identified can be found in Error! Reference source not found. something is missing here

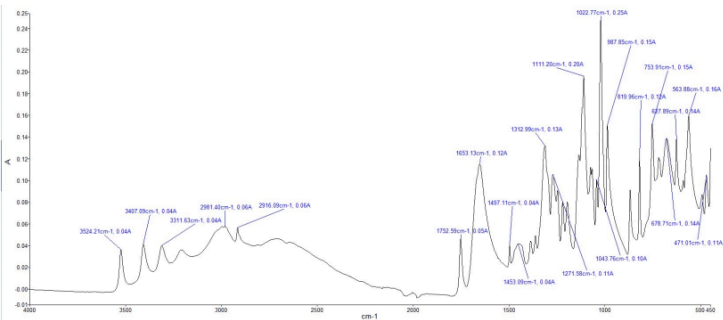


Figure 1 Sample A

Table 1 Sample A Identified peaks

Peak Wavenumber	Amplitude	Possible bonds	note
3524	0.04	O-H / N-H	Broad peak between 3550-2000cm ⁻¹
3407	0.04	O-H / N-H	
3312	0.04	O-H / N-H / O-H / C-H / =C-H	
2981	0.06	O-H / N-H / C-H	
1753	0.05	C-H / C=O	sharp separate peak
1653	0.12	C-H / C=O / C=N / C=C / N-H	Mostly sharp peak
1497	0.04	N-O / C=H	Smaller peaks with bases merging
1453	0.04	C-H / O-H	
1313	0.13	O-H / C-F / S=O / C-N / C-O	Larger peak with bases merging further
1272	0.11	C-F / C-N / C-O	
1111	0.20	C-F / C-N / C-O	Sharp peak
1023	0.25	C-F / C-N / S=O / CO-O-CO	Largest peak detected on spectra very narrow

1044	0.10	C-F / C-N / C-O/ S=O/ CO-O-CO	Small peak between lulls of surrounding large peak
988	0.15	C-F / C=C/ =C-H	Sharp narrow peak
820	0.12	C=C / C-H / C-Cl	large sharp peak
753	0.15	C-H/ C-Cl	Several peaks with bases merged.
679	0.14	C=C / C-H / C-Br / C-Cl	
628	0.14	C-Br/ C-Cl	
564	0.16	C-Br / C-I / C-Cl/ M-O	
471	0.11	M-O	Smaller peak

In ascorbic acid there is several types of functional groups as can be seen in Figure 2. There is Hydroxyl groups (-OH), Carbonyl group (-C=O) and an cyclic ether group (lactone) (-O-), these have the following IR response:

Table 2 Ascorbic acid functional groups

Functional Group	IR Band	Notes	Presence
Hydroxyl (carboxylic acid)	3000-2500 [1]	Broad stretch	Yes
Carbonyl	1780-1710		Yes
Lactone	3600-3000; 1750-1730; 1200-1000		Yes

From the functional groups above as well as the similarity of the reference spectra (Figure 3) it is likely that the sample A is ascorbic acid.

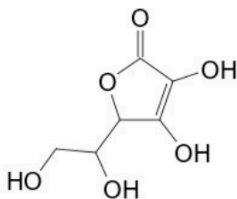


Figure 2 Ascorbic Acid Structure

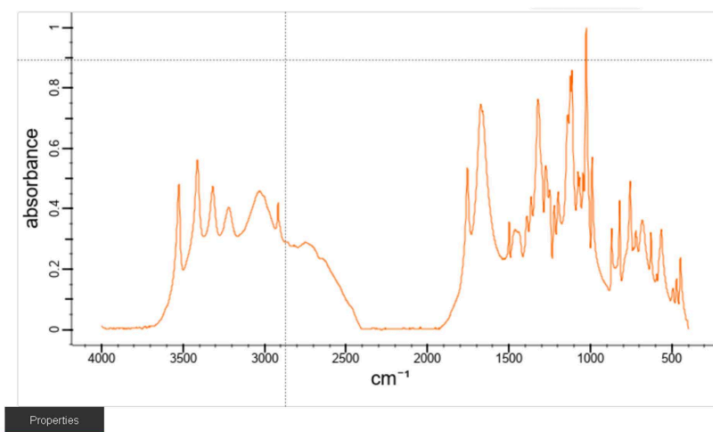


Figure 3 Ascorbic Acid Reference Spectra [2]

Sample B

Error! Reference source not found. shows the spectrum of sample B. The peaks identified can be seen in Table 3.

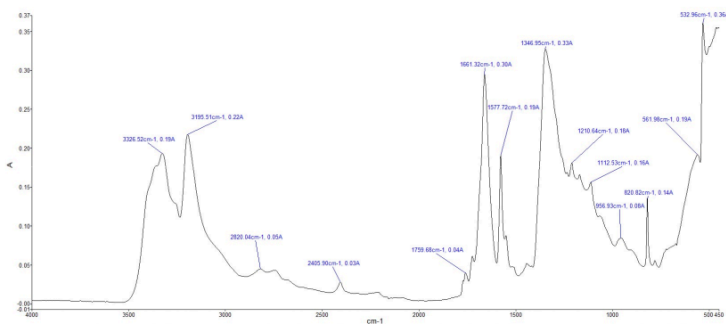


Figure 4 Sample B spectra

Table 3 Sample B Peaks

Peak Wavenumber	Amplitude	Possible Bonds	Notes
3327	0.19	O-H / N-H / C-H / =C-H	Large peaks with merged base
3196	0.22	O-H	
2820	0.05	O-H / N-H / C-H	Very small peaks over wide area, almost negligible
2406	0.03	-	
1760	0.04	C-H / C=O	Sharp peak
1661	0.30	C-H / C=O / C=N / C=C / N-H	
1578	0.19	N-H / C=C	Sharp peak
1347	0.33	O-H / C-F / S=O / C-N	Large peak with merged base
1211	0.18	C-F / C-O / C-N	Smaller peak with merged base
1112	0.16	C-F / C-N / C-O	
957	0.08	=C-H / C=C	Small peak wide base
821	0.14	C=C / C-H / C-Cl	Sharp peak
562	0.19	C-Br / C-I / C-Cl M-O	Large peaks with wide base
533	0.36	C-Br / C-I / C-Cl / M-O	



The functional groups of guanidine nitrate are as follows: amino group (NH₂) primary amine / (NH) secondary amine with two NH₂ groups and a single NH group.

Table 4 Guanidine Nitrate functional groups

Functional group	IR response	notes	Presence
Primary Amine	3400-3500 [3]	Two distinct peaks	Yes
Secondary Amine	3420	Single peak	Possible

Table 4 shows that the NH₂ group can be seen, but that the secondary amine is mostly hidden by the primary amine, as there is significant overlap in the IR response. When comparing the spectra recorded with the reference spectra (Figure 6) it can be seen that these is a good match. Therefore sample B is likely Guanidine nitrate.

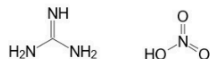


Figure 5 Guanidine Nitrate structure

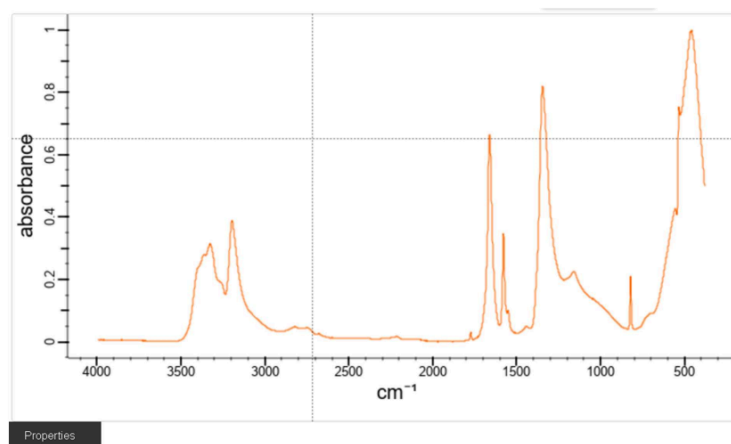


Figure 6 Guanidine Nitrate Reference Spectra [4]

Sample C

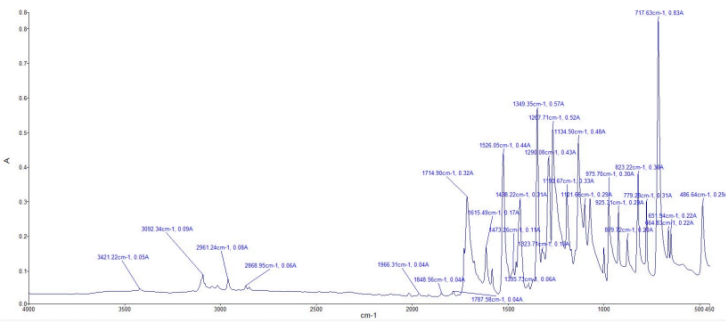


Figure 7 Sample C Spectra

Peak Wavenumber	Amplitude	Potential Bonds	Notes
3421	0.05	O-H	Small narrow peaks
3092	0.09	C-H / O-H	
2961	0.08	O-H / N-H / C-H	
2869	0.06	O-H / N-H / C-H	
1966	0.04	C=C=C / C=C=N / C-H	
1848	0.04	C-H / C=O	
1788	0.04	C-H / C=O	
1715	0.32	C-H / C=O	large sharp peaks
1615	0.17	C=O / C=C / N-H / C=C	
1526	0.44	N-O	
1473	0.11	C-H	
1438	0.31	C-H / O-H	
1396	0.05	C-H / O-H / S=O / C-F	
1324	0.16	O-H / C-F / S=O / C-N / C-O	
1349	0.57	O-H / C-F / S=O / C-N	
1290	0.43	C-F / O-H / S=O / C-N / C-O	
1268	0.52	C-F / C-N / C-O	
1193	0.33	C-F / C-O / C-N	
1134	0.48	C-F / C-N / C-O	

1102	0.29	C-F/C-N/C-O	
976	0.30	C=C / =C-H	
925	0.29	=C-H	
880	0.20	C=C/ C-H	
823	0.38	C=C/C-H C-Cl	
778	0.31	C=C / C-H/ C-Cl	
718	0.83	C=C / C-H/ C-Cl	
665	0.22	C=C/C-H/C-Br/C-Cl	
652	0.22	C=C/ C-H/ C-Br/ C-Cl	
487	0.29	C-I / M-O	

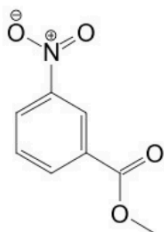
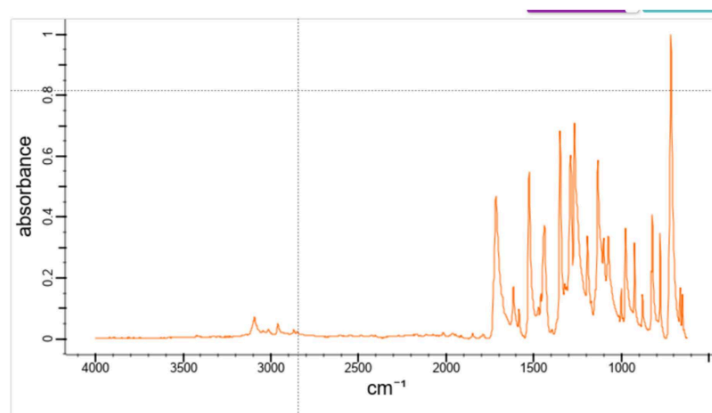


Figure 8 Methyl 3-nitrobenzoate structure

Table 5 Methyl 3 Nitrobenzoate functional groups

Functional group	IR response	notes	Presence
Ester Group	2950 1735-1750, 1200-1300	Sharp prominent peak	Yes
Nitro Group	1500-1570, 1300-1370	Two distinct strong peaks	Yes
Aromatic Ring	~3030, 1450-1600, 690-900	Multiple smaller peaks	Yes

From the available information of both the functional groups, and the reference spectra it is highly likely that sample 3 is Methyl 3 Nitrobenzoate. Literature describes a large number of peaks present at the lower end of the spectra, with only weak peaks present in the $\sim 3000\text{cm}^{-1}$ range. These are all present, showing a good match.



Properties

Figure 9 Methyl 3 nitrobenzoate reference spectra [5]

Sample D

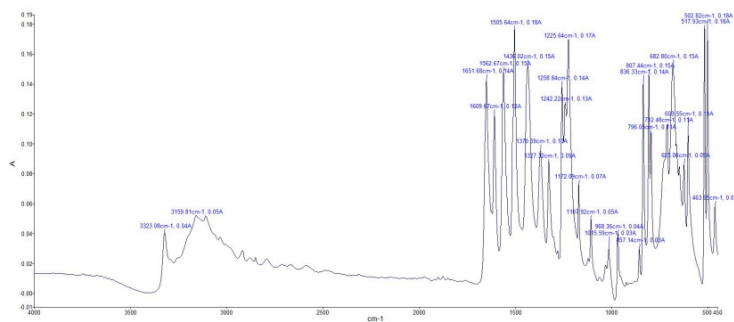


Figure 10 Sample D spectra

Peak Wavenumber	Amplitude	Possible bonds	Notes
3323	0.04	O-H / N-H / C-H / C-H	Broad shallow peaks
3160	0.05	O-H	
1652	0.14	C-H / C=O / C=N / C=C / N-H	Sharp tall peaks
1610	0.12	C=O / C=C / N-H	
1563	0.15	N-H / C=C / N-O	
1506	0.18	N-O / C-H	
1436	0.15	C-H / O-H	
1371	0.10	C-H / O-H / S=O / C-F	
1327	0.09	O-H / C-F / S=O / C-N / C-O	
1259	0.14	C-F / C-N / C-O	
1242	0.13	C-F / C-O / C-N	
1225	0.17	C-F / C-O / C-N	
1172	0.07	C-F / C-N / C-O	
1107	0.05	C-F / C-N / C-O	
1016	0.03	C-F / C-N / S=O	
968	0.04	C=C / C-H	
857	0.03	C=C / C-H / C-Cl	
836	0.14	C=C / C-H / C-Cl	
807	0.15	C=C / C-Cl / C-H	
796	0.11	C=C / C-H / C-Cl	
712	0.11	C=C / C-H / C-Cl	
683	0.15	C=C / C-H / C-Br / C-Cl	
625	0.09	C-Br / C-Cl	
604	0.11	C-Br / C-I / C-Cl / M-O	
518	0.18	C-Br / C-I / M-O	
502	0.18	C-Br / C-I / M-O	
464	?	M-O	



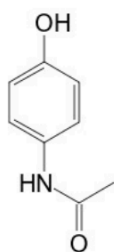


Figure 11 Acetaminophen structure

Table 6 Acetaminophen functional groups

Functional group	IR response	notes	Presence
Hydroxyl Group (phenol)	3200-3550	Large broad stretch	Yes
Amide Group	3300-3400, 1640-1680, 1500-1600	Medium peak, strong peak, multiple strong peaks	Yes
Aromatic Ring	~3030, 1500-1600, 700-900	Weak peaks, smaller peaks, present in fingerprint zone.	Yes

All evidence present is highly indicative of the presence of acetaminophen; the functional groups show a good match as well as the reference spectra. Therefore, the author has high confidence that sample D is likely acetaminophen (paracetamol).

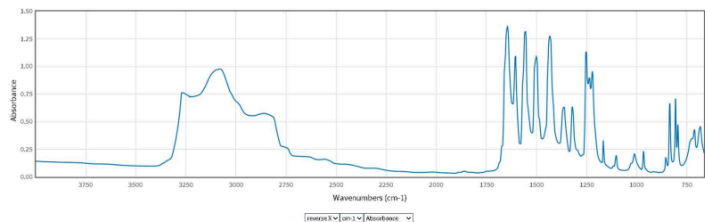


Figure 12 Acetaminophen reference spectra [6]

Conclusions

In Conclusion, FTIR has been used to identify all 4 compounds. Three of the four present near perfect matches with the available literature, with only sample 2, presenting a challenge when identifying the functional groups; but still showing a good match with the reference spectra.

FTIR is an excellent confirmatory method, that allows rapid identification of existing compounds when using libraries whilst also providing opportunities to identify new compounds from the basic principles of the bonds which make up all matter.

References

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] SPEC. [Accessed 15 10 2025].

Engagement with Literature 9/15

Good use of reference spectra and basic peak tables but no sources mentioned. Sources are relevant and mostly correctly formatted in IEEE style. However, several peak assignments are not explicitly linked to literature within the text, and vibrational ranges are sometimes presented without citation. Engagement is solid but mainly descriptive rather than analytical.

Knowledge and Understanding 13/20

You demonstrate basic understanding of FT-IR principles and functional groups for all four samples. However, vibrational modes (stretching, bending, twisting etc.), the basis of IR absorption, are not described. The introduction focuses on identification rather than the actual aim: producing a reproducible FT-IR method. Functional-group identification on spectra would add clarity and help readers understand your assignments.

Cognitive and Intellectual Skills 13/20

Sample identification is correct and supported with reasonable explanation. You use reference spectra well and apply selective reasoning (especially for nitro and aromatic functional groups). However, analysis remains partly descriptive, peak tables list many possible bonds rather than focusing on chemically relevant ones, and fingerprint-region interpretation is limited. More direct comparison to literature values would improve analytical depth.

Practical Skills 12/30

This is the main weakness. The written method is incomplete and does not contain all the critical FT-IR parameters needed for reproducibility. Missing details include: correct spectral range (written as 4000–4450 cm⁻¹, should be 4000–450 cm⁻¹) resolution apodisation baseline/smoothing settings ATR correction atmospheric suppression scan speed detector and beam splitter details QC criteria (background quality, S/N checks, repeat-scan rules) sample-handling guidance Some of these appear only in the screenshot at the end, but they must be included in the method itself. This significantly reduces marks in the practical skills category.

Transferable Skills 10/15

Clear layout, good use of chemical structures and labelled figures. Writing is mostly formal and easy to follow. Some duplicated figures and very long tables reduce clarity. The key methodological information should be integrated into the main body rather than placed only in a scan.

57 /100

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PAGE 4

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