

**STUDY OF PLASTIC SOLID ACCELERANT USING
FOURIER TRANSFORM INFRARED (FTIR)
SPECTROSCOPY ANALYSIS AND CHEMOMETRIC
ANALYSIS**

HABIBAH BINTI ABDUL SUKOR

UNIVERSITI SAINS MALAYSIA

2026

**STUDY OF PLASTIC SOLID ACCELERANT USING
FOURIER TRANSFORM INFRARED (FTIR)
SPECTROSCOPY ANALYSIS AND CHEMOMETRIC
ANALYSIS**

by

HABIBAH BINTI ABDUL SUKOR

**Dissertation submitted in partial fulfilment of the requirements for the degree
of Bachelor Science in Forensic Science (Honours)**

February 2026

CERTIFICATE

This is to certify that the dissertations entitled "**STUDY OF PLASTIC SOLID ACCELERANT USING FOURIER TRANSFORM INFRARED (FTIR) SPECTROSCOPY ANALYSIS AND CHEMOMETRIC ANALYSIS**" is the bona fide record of research work done by Ms. "**HABIBAH BINTI ABDUL SUKOR**". During the period of October 2025 to February 2026 under my supervision. I have read this dissertation and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality as a dissertation to be submitted in partial fulfilment for the degree of Bachelor of Sciences (Honours) Forensic Science.

Main supervisor,



CHM. DR. WAN NUR SYUHAILA BINTI MAT DESA

Lecturer,

Forensic Science Programme,

School of Health Science,

Universiti Sains Malaysia,

16150 Kubang Kerian,

Kelantan Darul Naim.

Date: **1.2.2026**

DECLARATION

I hereby declare that this thesis is the result of my own investigation, except where otherwise stated that and duly acknowledge. I also declared that it has not been previously or concurrently submitted as a whole for any other degrees at Universiti Sains Malaysia or other institutions. I grant Universiti Sains Malaysia the right to use the dissertation for teaching and promotional purposes.

Signature:

.....

HABIBAH BINTI ABDUL SUKOR

Date: 31/1/2026

ACKNOWLEDGEMENT

First and foremost, I humbly express my deepest gratitude to Allah for granting me strength, good health and perseverance to complete this final year project research. Without His blessings, this work would not have been possible.

Moreover, I would like to sincerely thank my supervisor, ChM. Dr. Wan Nur Syuhaila Binti Mat Desa, for her continuous guidance, support and valuable advice throughout the course of this research. Her patience, encouragement and constructive feedback greatly contributed to the successful completion of this study. I would also like to express my appreciation to ChM. Dr. Dzulkiflee Bin Ismail for his assistance, guidance and knowledge shared during completing this research. My sincere thanks are also extended to all lecturers of the Forensic Science Programme for their teaching, support and contribution to my academic development.

I am deeply grateful to my parents and family for their endless prayers, belief and moral support throughout my academic journey. Their encouragement has been a constant source of strength and motivation for me. I would also like to thank my friends for always listening to my problems, offering encouragement and showing empathy during challenging times. Lastly, I would like to express my heartfelt appreciation to my fiancé for his continuous motivation, understanding and reminders to stay focused and complete my work.

Alhamdulillah.

TABLE OF CONTENTS

ACKNOWLEDGEMENT	v
TABLE OF CONTENTS.....	vi
LIST OF FIGURES	viii
LIST OF TABLES.....	x
LIST OF ABBREVIATIONS	xi
LIST OF SYMBOLS	xii
ABSTRAK	xiii
ABSTRACT	xiv
CHAPTER 1: INTRODUCTION	1
1.1 Background of the Study.....	1
1.2 Problem Statement	4
1.3 Objective	5
1.3.1 General Objective.....	5
1.3.2 Specific Objective	5
1.4 Research Questions.....	5
1.5 Significance of Study.....	6
CHAPTER 2: LITERATURE REVIEW	7
2.1 Arson	7
2.2 Ignitable Liquid	8
2.2.1 Petrol	12
2.3 Plastics	13
2.3.1 Plastics in Fire Scenes	16
2.4 Fourier Transform Infrared Spectroscopy (FTIR).....	18
2.4.1 FTIR Analysis of Plastic Products	20
2.5 Chemometric Analysis	24
CHAPTER 3: METHODOLOGY	25
3.1 Sample Collection	25
3.2 Sample Preparation	29
3.3 FTIR Analysis of Unburnt Plastics	29
3.4 Burning Procedure	30
3.5 FTIR Analysis of Burnt Plastics	31
3.6 Addition of Petrol and FTIR Analysis of Petrol-Exposed Burnt Plastics	31
3.7 Data Analysis	32
CHAPTER 4: RESULT AND DISCUSSION	33

4.1 FTIR Spectrum Interpretation	33
4.1.1 Unburnt Plastic Samples	33
4.1.2 Burnt Plastic Samples	43
4.1.3 Burnt Plastic Samples Exposed to Petrol	62
4.2 Principal Component Analysis (PCA) Interpretation	81
4.2.1 Unburnt Plastic Samples	82
4.2.2 Burnt Plastic Samples	83
4.2.3 Burnt Plastic Samples Exposed to Petrol	84
CHAPTER 5: CONCLUSION AND RECOMMENDATIONS.....	86
5.1 Conclusion.....	86
5.2 Limitations of The Study	87
5.3 Recommendations for Future Work.....	88
REFERENCES	89
APPENDICES	94
Appendix A: FTIR Spectra of Unburnt Plastic Samples	94
Appendix B: FTIR Spectra of Burnt Plastic Samples	104
Appendix C: FTIR Spectra of Burnt Plastic Samples Exposed to Petrol	114
Appendix D: Overlay FTIR Spectra of Representative Plastic Samples Under Different Conditions.....	124

LIST OF FIGURES

Figure 2.1: Example of a gasoline pattern; 50 % evaporated gasoline (ASTM E1618, 2019).	12
Figure 2.2: Fractional distillation of crude oil (Baheti, 2025).	15
Figure 2.3: Mid-IR spectrum region (Nandiyanto et al., 2019).	20
Figure 2.4: Example of the FTIR spectra of the six most used industrial plastics (Villegas-Camacho et al., 2024)	21
Figure 3.1: Bruker Alpha II Compact FT-IR Spectrometer.....	29
Figure 4.1: Representative FTIR spectrum of unburnt PET, plastic bottle (P01).	34
Figure 4.2: Representative FTIR spectrum of unburnt PE, adhesive wall sticker (P05).	35
Figure 4.3: Representative FTIR spectrum of unburnt PVC, vinyl floor sticker (P03).	36
Figure 4.4: Representative FTIR spectrum of unburnt PP, plastic woven mat (P07).	37
Figure 4.5: Representative FTIR spectrum of unburnt PS, plastic spoon (P10).	38
Figure 4.6: Representative FTIR spectrum of unburnt PC, electrical plug housing (P11).	39
Figure 4.7: Representative FTIR spectrum of unburnt PU, phone case (P18).	40
Figure 4.8: Representative FTIR spectrum of unburnt IIR, tire tube (P15).	41
Figure 4.9: Representative FTIR spectrum of unburnt VIS, viscose fibre (P19).	42
Figure 4.10: Representative FTIR spectrum of burnt PET, plastic bottle (P01).	44
Figure 4.11: Overlay of FTIR spectra of unburnt PET and burnt PET samples.	44
Figure 4.12: Representative FTIR spectrum of burnt PE, adhesive wall sticker (P05).	46
Figure 4.13: Overlay of FTIR spectra of unburnt PE and burnt PE samples.	46
Figure 4.14: Representative FTIR spectrum of burnt PVC, vinyl floor sticker (P03).	48
Figure 4.15: Overlay of FTIR spectra of unburnt PVC and burnt PVC samples.	48
Figure 4.16: Representative FTIR spectrum of burnt PP, plastic woven mat (P07).	50
Figure 4.17: Overlay of FTIR spectra of unburnt PP and burnt PP samples.	50
Figure 4.18: Representative FTIR spectrum of burnt PS, plastic spoon (P10).	52
Figure 4.19: Overlay of FTIR spectra of unburnt PS and burnt PS samples.	52
Figure 4.20: Representative FTIR spectrum of burnt PC, electrical plug housing (P11).	54
Figure 4.21: Overlay of FTIR spectra of unburnt PC and burnt PC samples.	54
Figure 4.22: Representative FTIR spectrum of burnt PU, phone case (P18).	56
Figure 4.23: Overlay of FTIR spectra of unburnt PU and burnt PU samples.	56
Figure 4.24: Representative FTIR spectrum of burnt IIR, tire tube (P15).	58
Figure 4.25: Overlay of FTIR spectra of unburnt IIR and burnt IIR samples.	58
Figure 4.26: Representative FTIR spectrum of burnt VIS, viscose fabric (P19).	60
Figure 4.27: Overlay of FTIR spectra of unburnt VIS and burnt VIS samples.	60
Figure 4.28: Representative FTIR spectrum of burnt-petrol PET, plastic bottle (P01).	63

Figure 4.29: Overlay of FTIR spectra of burnt PET and burnt-petrol PET samples.....	63
Figure 4.30: Representative FTIR spectrum of burnt-petrol PE, adhesive wall sticker (P05).	65
Figure 4.31: Overlay of FTIR spectra of burnt PE and burnt-petrol PE samples.	65
Figure 4.32: Representative FTIR spectrum of burnt-petrol PVC, vinyl floor sticker (P03)....	67
Figure 4.33: Overlay of FTIR spectra of burnt PVC and burnt-petrol PVC samples.....	67
Figure 4.34: Representative FTIR spectrum of burnt-petrol PP, plastic woven mat (P07). ...	69
Figure 4.35: Overlay of FTIR spectra of burnt PP and burnt-petrol PP samples.	69
Figure 4.36: Representative FTIR spectrum of burnt-petrol PS, plastic spoon (P10).....	71
Figure 4.37: Overlay of FTIR spectra of burnt PS and burnt-petrol PS samples.	71
Figure 4.38: Representative FTIR spectrum of burnt-petrol PC, electrical plug housing (P11).	73
Figure 4.39: Overlay of FTIR spectra of burnt PC and burnt-petrol PC samples.....	73
Figure 4.40: Representative FTIR spectrum of burnt-petrol PU, phone case (P18).	75
Figure 4.41: Overlay of FTIR spectra of burnt PU and burnt-petrol PU samples.....	75
Figure 4.42: Representative FTIR spectrum of burnt-petrol IIR, tire tube (P15).	77
Figure 4.43: Overlay of FTIR spectra of burnt IIR and burnt-petrol IIR samples.....	77
Figure 4.44: Representative FTIR spectrum of burnt-petrol VIS, viscose fabric (P19).	79
Figure 4.45: Overlay of FTIR spectra of burnt VIS and burnt-petrol VIS samples.	79
Figure 4.46: PCA of unburnt plastic samples.....	82
Figure 4.47: PCA of burnt plastic samples.....	83
Figure 4.48: PCA of burnt plastic samples exposed to petrol.....	84

LIST OF TABLES

Table 2.1: NFPA classifications for flammable and combustible liquids (Robin Zevotek, 2024).	9
Table 2.2: Ignitable liquid classification scheme with examples of known products for each class (ASTM E1618, 2019).	10
Table 2.3: Major ions present in mass spectra of common ignitable liquids (ASTM E1618, 2019).	11
Table 2.4: Main polymer types, monomers, its chemical structure (Baheti, 2025).	14
Table 3.1: List of Plastic Samples Collected for Analysis.	25
Table 4.1: Characteristic FTIR absorption bands of unburnt PET samples.	34
Table 4.2: Characteristic FTIR absorption bands of unburnt PE samples.	35
Table 4.3: Characteristic FTIR absorption bands of unburnt PVC samples.	36
Table 4.4: Characteristic FTIR absorption bands of unburnt PP samples.	37
Table 4.5: Characteristic FTIR absorption bands of unburnt PS samples.	38
Table 4.6: Characteristic FTIR absorption bands of unburnt PC samples.	39
Table 4.7: Characteristic FTIR absorption bands of unburnt PU samples.	40
Table 4.8: Characteristic FTIR absorption bands of unburnt IIR samples.	41
Table 4.9: Characteristic FTIR absorption bands of unburnt VIS sample.	42
Table 4.10: List of spectral changes of PET samples after burning.	45
Table 4.11: List of spectral changes of PE samples after burning.	47
Table 4.12: List of spectral changes of PVC samples after burning.	49
Table 4.13: List of spectral changes of PP samples after burning.	51
Table 4.14: List of spectral changes of PS samples after burning.	53
Table 4.15: List of spectral changes of PC samples after burning.	55
Table 4.16: List of spectral changes of PU samples after burning.	57
Table 4.17: List of spectral changes of IIR samples after burning.	59
Table 4.18: List of spectral changes of VIS samples after burning.	61
Table 4.19: List of spectral changes of burnt PET samples after petrol exposure.	64
Table 4.20: List of spectral changes of burnt PE samples after petrol exposure.	66
Table 4.21: List of spectral changes of burnt PVC samples after petrol exposure.	68
Table 4.22: List of spectral changes of burnt PP samples after petrol exposure.	70
Table 4.23: List of spectral changes of burnt PS samples after petrol exposure.	72
Table 4.24: List of spectral changes of burnt PC samples after petrol exposure.	74
Table 4.25: List of spectral changes of burnt PU samples after petrol exposure.	76
Table 4.26: List of spectral changes of burnt IIR samples after petrol exposure.	78
Table 4.27: List of spectral changes of burnt VIS samples after petrol exposure.	80

LIST OF ABBREVIATIONS

ASTM	American Society for Testing and Materials
CD	Compact Disc
EIP	Extracted Ion Profiling
ETBE	Ethyl tert-butyl ether
FTIR	Fourier Transform Infrared Spectroscopy
GC–MS	Gas Chromatography–Mass Spectrometry
HCA	Hierarchical Cluster Analysis
HDPE	High-Density Polyethylene
IIR	Butyl-Rubber
IL	Ignitable Liquid
ILR	Ignitable Liquid Residue
IR	Infrared
JBPM	Jabatan Bomba dan Penyelamat Malaysia
LDPE	Low-Density Polyethylene
LDA	Linear Discriminant Analysis
MTBE	Methyl tert-butyl ether
NFPA	National Fire Protection Association
PCA	Principal Component Analysis
PC	Polycarbonate
PDRM	Polis Diraja Malaysia
PE	Polyethylene
PET	Polyethylene Terephthalate
PP	Polypropylene
PS	Polystyrene
PU	Polyurethane
PVC	Polyvinyl Chloride
RON	Research Octane Number
SIMCA	Soft Independent Modelling of Class Analogy
SPSS	Statistical Package for the Social Sciences
VIS	Viscose
VOC	Volatile Organic Compound

LIST OF SYMBOLS

°C	Degree Celsius
cm	Centimetre
cm ⁻¹	Wavenumber
μL	Microlitre
m/z	Mass-to-charge ratio
%	Percentage

ABSTRAK

Plastik lazimnya terdapat di tempat kebakaran dan berpotensi bertindak sebagai pemecut pepejal kerana sifatnya yang mudah terbakar, sekali gus mempengaruhi tingkah laku kebakaran dan tafsiran forensik. Kajian ini dijalankan untuk mengkaji kelakuan produk plastik terpilih di bawah keadaan berkaitan kebakaran menggunakan Spektroskopi Inframerah Transformasi Fourier (FTIR) yang digabungkan dengan analisis kemometrik iaitu Analisis Komponen Utama (PCA). Sebanyak 20 sampel plastik dianalisis menggunakan FTIR bagi mendapatkan spektrum asas plastik yang masih belum dibakar. Sampel-sampel tersebut kemudiannya dibakar secara terkawal dalam tempoh masa yang telah ditetapkan. Kemudian, analisis FTIR dijalankan terhadap sampel plastik yang telah dibakar tersebut. Seterusnya, sejumlah kecil petrol diletakkan di atas sampel plastik yang telah dibakar dan analisis FTIR selanjutnya dijalankan bagi menilai kesan pendedahan pemecut. Spektrum FTIR yang diperoleh daripada sampel yang masih belum dibakar, dibakar dan didedahkan dengan petrol telah ditafsir, dicirikan dan dibandingkan untuk mengenal pasti jenis polimer serta perubahan dalam kumpulan fungsi dan corak spektrum. PCA kemudiannya diaplikasikan ke atas kawasan cap jari spektrum FTIR bagi memvisualisasikan tingkah laku pengelompokan antara sampel. Hasil kajian menunjukkan bahawa sampel plastik mempamerkan ciri spektrum yang khusus bagi setiap polimer. Perkara ini membolehkan pengelompokan produk plastik berdasarkan jenis polimer. Di samping itu, pembakaran dan pendedahan kepada petrol menyebabkan perubahan spektrum berlaku; namun demikian, ciri spektrum utama masih dapat dikesan, sekali gus membolehkan pengecaman jenis polimer terhadap produk plastik tersebut.

ABSTRACT

Plastics are commonly present at fire scenes and may act as solid accelerants due to their combustible nature, potentially influencing fire behaviour and forensic interpretation. This study investigated the behaviour of selected plastic products under fire-related conditions using Fourier Transform Infrared Spectroscopy (FTIR) combined with chemometric analysis through Principal Component Analysis (PCA). A total of 20 plastic samples were analyzed using FTIR to obtain baseline spectra of unburnt materials. The samples were then subjected to controlled burning for a fixed duration, followed by FTIR analysis of the burnt residues. Subsequently, a small volume of petrol was applied to the burnt samples and further FTIR analysis was performed to evaluate the effects of accelerant exposure. The FTIR spectra obtained from unburnt, burnt and petrol-exposed samples were interpreted, characterized and compared to assess polymer types as well as changes in functional groups and spectral patterns. PCA was then applied to the FTIR fingerprint region to visualize clustering behaviour among the samples. The results of this study showed that plastic samples exhibited polymer-specific spectral features, allowing grouping based on polymer type. In addition, burning and petrol exposure caused observable spectral changes; however, their characteristic spectral features remained detectable, enabling identification of the polymer type.

CHAPTER 1

INTRODUCTION

1.1 Background of the Study

Fire is an exothermic chemical reaction that releases energy in the form of heat and light when combustible material rapidly oxidises (Daeid, 2004). For a fire to occur, certain conditions must be fulfilled, which can be explained using established fire models. The fire triangle model is the earliest model that describes combustion and states that fire occurs when three essential elements which are heat, fuel and oxygen interact in the right proportions. The model was later expanded into the fire tetrahedron which introduces a fourth element representing the uninhibited chemical chain reaction that sustains the combustion process (Kadhom et al., 2023). By removing or interrupting any one of these components, fire suppression can be achieved.

From 2016 to 2023, the Fire and Rescue Department of Malaysia (JBPM) recorded thousands of fire incidents across the country with an average of 35,821 cases per year affecting residential, industrial and vehicle sectors. The report shows that 2019 had the highest number of fire cases with 50,613 incidents, while the number of cases gradually decreased in the following years, reaching the lowest count of 17,235 in 2023 (JBPM, 2023). These statistics highlight the frequent occurrence of fire incidents in Malaysia and reflect the operational burden on JBPM which must respond to a large number of fire-related emergencies. Efficient fire prevention strategies, rapid response capabilities and detailed fire investigation protocols are critical to minimise losses and ensure public safety.

There are three classifications of the cause of fire according to National Fire Protection Association (NFPA) 921 (2001), which are natural, accidental and incendiary fires. Natural fires occur due to natural phenomena without human intervention, such as earthquakes or lightning strikes. For accidental fires, it usually arises from unintentional human actions that

initiate or spread fire. Meanwhile, incendiary fires are deliberately ignited with the knowledge that the fire should not occur. To establish the cause, a systematic process such as forensic fire investigation is crucial to determine the origin, cause and development of a fire. It involves scientific principles to understand how the fire started, how it spread and whether external factors such as accelerant contributed to its behaviour.

The fire investigation process begins with site observation, which involves securing the area, ensuring safety and conducting a preliminary examination to identify burn patterns and possible sources of ignition. The fire scene is then documented through notes, sketches and photographs before the evidence is collected and preserved under appropriate conditions while maintaining the chain of custody to protect its integrity and admissibility in court. In addition, witnesses are interviewed to obtain relevant information about the incident. After that, a crucial step involving the analysis of fire scene findings is conducted, requiring detailed and precise examination. Then, the findings are compiled into a report and presented as part of the investigation outcome (Elmore, 2024).

In Malaysia, fire investigations are mainly investigated by JBPM, or “Bomba”, together with the Royal Malaysia Police (PDRM). JBPM acts as the lead investigative authority, focusing on determining the origin and cause of a fire through systematic and scientific procedures. Their work includes identifying the source, cause and circumstances of the incident, followed by recommendations to improve fire prevention and firefighting efficiency (JPBM, 2021). In cases where the fire is suspected to involve criminal elements such as arson, murder or suicide, the investigation is handed over to PDRM, who works in collaboration with JBPM. The forensic findings prepared by JBPM will serve as scientific evidence to support PDRM’s legal investigations and subsequent prosecution in court (The Vibes, 2025).

Usually, detection and identification of ignitable liquid residues (ILRs) are important pieces of evidence in forensic fire investigations to determine whether a fire was accidental or

intentionally set. In many incendiary fires such as arson, arsonists often use ignitable liquids (ILs) as accelerants to initiate the fire and accelerate the spread of fire. These liquids are commonly used due to their high volatility and flammability, which allow them to burn quickly and intensely, thereby causing extensive damage. Petroleum-based products such as petrol, diesel and kerosene are often used ILs due to their wide availability and ease of access as they can be bought from market or gas stations (Ferreiro-González et al., 2016). Thus, the presence of ILRs in the fire debris can provide important clues and strong evidence of arson.

However, ILs are not the only materials capable of initiating or enhancing a fire. Accelerants may exist in liquid, gaseous or solid forms (Banyal, 2023). In real fire scenes, a wide range of combustible materials, including plastics, wood, wax and textiles may be present. When deliberately introduced or arranged, these materials can function as solid accelerants, defined as combustible solid substrate intentionally used to initiate or sustain fire spread. During combustion, such substrate may melt and exhibit liquid-like behaviour, generating pyrolysis products that resemble the behaviour of ILs (Falatová et al., 2021). Therefore, solid accelerants can increase the rate and intensity of a fire by prolonging fuel availability, particularly when present in bulk.

The residue of the solid substrates at a fire scene can be analysed for the detection of any ILRs or to evaluate the contribution of the solid material itself to fire initiation. In cases where solid materials, particularly plastics, may mimic the presence of accelerants or when laboratories require fast comparative results, Fourier Transform Infrared (FTIR) spectroscopy provides a useful preliminary analytical approach. FTIR is widely used in polymer characterisation due to its rapid, minimal sample preparation and non-destructive analysis. It identifies molecular structures based on vibrational behaviour of atoms within a molecule allowing specific functional groups and chemical bonds to be detected (Nandiyanto et al., 2023). Thus, FTIR can function as an effective initial screening tool for solid accelerants.

1.2 Problem Statement

In forensic fire investigation, the accurate detection and identification of ILRs are crucial for determining whether a fire was accidental or deliberate. However, not all fires involve the use of ILs, as solid materials may also be intentionally introduced or arranged to initiate or sustain combustion. Plastics are commonly present in fire scenes and can function as solid accelerants due to their ability to soften, melt and drip upon heating, forming oil pool-like or wall-like flames that accelerate flame propagation, enlarge the burning area and increase fire hazards (Chen et al., 2023). Moreover, most common plastics consist of long carbon-hydrogen polymer chains similar to ILs and undergo pyrolysis when exposed to heat (Zang et al., 2024), allowing them to behave as accelerant and enhance fire spread.

Given the widespread presence of plastics in modern environments, there is limited research that systematically examines their role as solid accelerants. In particular, there is a lack of comparative data on the FTIR profiles of unburnt plastics, burnt plastics and burnt plastics subsequently exposed to petrol. This creates a significant gap in current forensic studies on understanding of how different plastic types behave as solid accelerants and how their chemical signatures evolve under fire-related conditions. Therefore, this study aims to examine the FTIR spectral behavior of selected plastic products before burning, after burning and following petrol exposure.

1.3 Objective

1.3.1 General Objective

1. To study the FTIR spectral characteristics of selected plastic products before burning, after burning and after petrol exposure, in order to understand the behaviour of plastic solid accelerants in fire-related cases.

1.3.2 Specific Objective

1. To characterise the FTIR spectra of selected unburnt plastic products.
2. To evaluate changes in FTIR spectra of plastics after burning, with and without petrol exposure.
3. To apply chemometric analysis to analyse FTIR spectral data of unburnt, burnt and burnt with petrol-exposed plastic samples.

1.4 Research Questions

1. What are the characteristic FTIR spectral features of the selected unburnt plastics?
2. How do the FTIR spectra of plastics change after burning, with and without petrol exposure?
3. How can chemometric analysis be applied to FTIR spectral data of unburnt, burnt and burnt with petrol-exposed plastic samples?

1.5 Significance of Study

This study is important in the field of forensic fire investigation as it enhances understanding of the role of plastic products as solid accelerants under fire conditions and their behaviour in FTIR analysis. Plastics are commonly present at fire scenes and have ability to melt, drip and undergo pyrolysis which can contribute to fire initiation and propagation in an accelerant-like manner. By analysing the FTIR spectral characteristics of unburnt, burnt and petrol-exposed plastics, this research provides insight into the chemical changes associated with plastic-based solid accelerants.

The findings of this study can serve as a reference for further research involving other types of polymers and varying fire-related conditions. The results may contribute to more accurate interpretation of fire debris evidence and support advancement in forensic fire debris analysis. Overall, this study will provide essential baseline spectral information that can assist future researchers and forensic laboratories in developing reliable reference databases and improving analytical protocols.

CHAPTER 2

LITERATURE REVIEW

2.1 Arson

Arson is a form of incendiary fire, which refers to the crime of intentionally starting a fire or explosion with malicious intent (NFPA 921, 2021). Arson can cause harm, damage property and may even be used to conceal evidence of other crime. In Malaysia, arson is governed under Act 574 of the Penal Code, with offenses classified under different sections depending on the intent and the type of property involved. Section 435 deals with mischief by fire or explosive substances resulting in damage of at least RM50, punishable by up to 14 years in prison and a fine. Section 436 applies to arson committed with the intent to destroy certain types of buildings such as houses or public facilities, with a potential punishment of up to 20 years in prison and a fine (Penal Code [Act 574], 2015).

In order to determine whether the fire is the result of arson, fire investigators need to analyse burn patterns, structural damage and other post-fire indicators to establish the origin and the cause of fire (O'Hagan & Banham, 2018). Several conditions related to fire behavior can provide physical evidence of intentional ignition. These include multiple points of origin, trailer-type fire patterns, the absence of an expected fuel load or ignition source, the presence of unusual fuel materials, burn injuries on a suspect and the discovery of incendiary devices (NFPA 921, 2021). In the examination of fire scene, the presence of these indicators increases the likelihood that the fire was deliberately set as in most accidental fires, such indicators would not typically be observed.

Arson remains a persistent problem in Malaysia. For example, in the 2017 Darul Quran Ittifaqiyah Madrasa fire, investigators detected petrol residues on multiple surfaces inside the building that has many combustible materials such as wooden cupboards and mattresses (Malay Mail, 2018). More recently, several arson incidents were reported in 2025, including

the Melaka case where a suspect threw a lit object into the compound, resulting in damage to a vehicle (The Sun Webdesk, 2025). In another 2025 case in Baling, Kedah, a suspect allegedly set fire to multiple properties and motorcycles due to a personal dispute (Zulkifli, 2025). These incidents demonstrate how fire investigators rely on indicators such as motive, physical evidence and burn patterns to determine whether a fire was intentionally set. Moreover, these cases highlight that beyond the initial ignition source, combustible substrates present at fire scenes can play a critical role in sustaining and influencing fire development.

2.2 Ignitable Liquid

Ignitable liquids (ILs) are defined as liquids that capable of fueling a fire. They can be also referred to as combustible or flammable liquids, depending on their flash points (NIST, 2025). In forensic science, ILs are commonly described as accelerants because they can be used to start or promote the spread of a fire. According to NFPA 921 (2021), an accelerant refers to any substance used to ignite fire or enhance the rate of degree of fire propagation. In the presence of an ignition source, the vapors released from ILs can ignite after mixing with air. These vapors can migrate from the original spill location, allowing ignition to occur at a point distant from where the liquid was deposited (Chubb, 2025).

Petroleum-based products are the most frequently encountered ILs in arson cases (Coulson & Morgan-Smith, 2000). Petroleum is a naturally occurring liquid composed mainly of hydrocarbons formed from the remains ancient marine organisms subjected to heat and pressure over millions of years (EIA, 2023). Its composition typically consists of 50-98% hydrocarbons, with the remaining portion made up of nitrogen, oxygen, sulphur, and trace metals (Moore & Ramamoorthy, 1984). Common petroleum-derived fuels such as petrol, diesel and kerosene which contain mixtures of volatile organic compounds (VOCs) are widely used as accelerants due to their high availability, low cost and ease of ignition for the purpose of intentional burning (Lim et al., 2018).

ILs are commonly classified based on their flash points and boiling points. The flash point refers to the lowest temperature at which a liquid releases sufficient vapor to form an ignitable mixture with air, indicating how easily it may catch fire. While boiling point is the temperature at which a liquid's vapor pressure equals to the surrounding atmospheric pressure, causing it to vaporise (Chubb, 2025). According to NFPA 30 (2021), flammable liquids have a closed-cup flash point below 37.8 °C, whereas combustible liquids have closed-cup flash point at or above this temperature. These parameters are essential for categorizing ILs, as listed in the Table 2.1.

Table 2.1: NFPA classifications for flammable and combustible liquids (Robin Zevotek, 2024).

Term	Class	Flash Point	Boiling Point
Flammable	Class IA	< 22.8°C	< 37.8°C
Flammable	Class IB	< 22.8°C	≥ 37.8°C
Flammable	Class IC	22.8-37.2°C	-
Combustible	Class II	37.8-59.4°C	-
Combustible	Class IIIA	60-92.8°C	-
Combustible	Class IIIB	≥ 93.3°C	-

American Society for Testing and Materials (ASTM) E1618 provides a standardised classification scheme for ILs to enhanced the identification of recovery ILs from fire debris. This system classifies ILs based on their boiling range and the distribution of hydrocarbons present in the product (Stauffer & Lentini, 2003). Using gas chromatography-mass spectrometry (GC-MS), seven major ILs classes can be distinguished. With the exception of gasoline, the remaining classes are further divided into light, medium and heavy subclasses according to their boiling ranges (ASTM E1618, 2019). The classification scheme for ILs is listed in the Table 2.2.

Table 2.2: Ignitable liquid classification scheme with examples of known products for each class (ASTM E1618, 2019).

Class	Light (C ₄ –C ₉)	Medium (C ₈ –C ₁₃)	Heavy (C ₉ –C ₂₀₊)
Gasoline — all brands (including gasohol and E85)	Fresh gasoline is typically in the range C ₄ –C ₁₂		
Petroleum Distillates (including de-aromatized)	Petroleum ether, cigarette lighter fluids, camping fuels, naphtha	Charcoal starters, paint thinners, dry cleaning solvents, mineral spirits, automotive parts cleaners, spray lubricants, lamp oils, deck sealers, varnishes, kerosene, insecticides	Kerosene, diesel fuel, charcoal starters, aviation fuels, insecticides, fuel additives, lamp oils, automotive parts cleaners
Isoparaffinic Products	Aviation gasolines, lighter fluids, charcoal starters	Charcoal starters, paint thinners, copier toners, mineral spirits, solvent cleaners, kerosene, lamp oils, gun oils	Spot cleaners, penetrating oils, insecticides
Aromatic Products	Automotive parts cleaners, solvent cleaners, xylenes, toluene-based products, lacquer thinners	Automotive parts cleaners, specialty cleaning solvents, insecticides, brush cleaners	Insecticides, adhesives
Naphthenic–Paraffinic Products	Cyclohexane-based solvents/products	Charcoal starters, insecticides, lamp oils, mineral spirits, automotive parts cleaners	Insecticides, lamp oils
Normal Alkane Products	-	Candle oils, copier toners, lamp oils, wax cleaners	Candle oils, lamp oil, carbonless forms, copier toners
Oxygenated Solvents	Alcohols, ketones, lacquer thinners, fuel additives, surface preparation solvents, automotive parts cleaners, spray adhesives, brush cleaners	Metal cleaners, gloss removers, degreasers, furniture strippers, cleaning solvents, insecticides	Biodiesels, fuel additives, floor finishes, insecticides
Others — Miscellaneous	Single component products, enamel reducers, lacquer thinners, aviation gasolines, racing gasolines	Turpentine products, mineral spirits, fuel additives, spray lubricants, brush cleaners, paint thinners, citrus cleaners, charcoal starters	Lamp oils, insecticides, citrus cleaners, automotive parts cleaners, kerosene, fuel additives

According to ASTM E1618 (2019), further data interpretation can be performed through extracted ion profiling (EIP), identification of specific compounds or combination of both. ILs generally contain six main categories of compounds which are normal alkanes, branched alkanes, cycloalkanes, aromatics, polynuclear aromatics and oxygenated compounds. While other compounds may appear in the chromatogram, they are typically not considered significant for interpretation. Each compound class produces its own set of characteristic ion fragments, which serve as useful marker during GC-MS analysis. These ions are listed in the Table 2.3.

Table 2.3: Major ions present in mass spectra of common ignitable liquids (ASTM E1618, 2019).

Compound Type	m/z
Alkane	43, 57, 71, 85, 99
Cycloalkane and alkene	55, 69
n-Alkylcyclohexanes	82, 83
Aromatic—alkylbenzenes	91, 105, 119, 92, 106, 120, 134
Indanes	117, 118, 131, 132
Alkyl naphthalenes (Condensed Ring Aromatics)	128, 142, 156, 170
Alkylstyrenes	104, 117, 118, 132, 146
Alkyl naphthacenes	178, 192, 206
Alkylbiphenyls/acenaphthenes	154, 168, 182, 196
Monoterpenes	93, 136
Ketones	43, 58, 72, 86
Alcohols	31, 45

2.2.1 Petrol

Petrol, also known as gasoline is a volatile and highly flammable liquid fuel derived from crude oil that commonly used in spark-ignited internal combustion engines to power vehicles such as cars and motorcycles (Britannica, 2025). Its composition is varies depending on the mixture of organic compounds produced through a multi-step refining processes and the type of crude oil used (Pavón et al., 2006) and often blended with additives to improve engine performance, reduce emissions and ensure stability. Petrol primarily consists of hydrocarbons, including alkanes in the C₄ to C₁₂ range, aromatic compounds such as alkylbenzenes, indanes and naphthalene, as well as oxygenated compounds such as ethanol, methyl tert-butyl ether (MTBE) and ethyl tert-butyl ether (ETBE) (Hendrikse et al., 2015).

Petrol is one of the most commonly used ILs to initiate and propagate a fire in incendiary fire cases. It has a low flash point, around 43 °C, allowing it to ignite easily from a spark or even minimal exposure to heat (Paula Coster, 2024). In addition, petrol also cheap, widely available and can be obtained without raising suspicion. Detection and identification of petrol is significant because it often leaves identifiable residues at the fire scene, typically showing an abundance of aromatic compounds with comparatively low levels of aliphatic (Stauffer & Lentini, 2003). Its complex mixture of hydrocarbons produces a highly distinctive chromatographic pattern, providing crucial evidence for forensic fire investigators (Stauffer et al., 2007). Figure 2.1 shown the example of gasoline pattern analyzed by GC-MS.

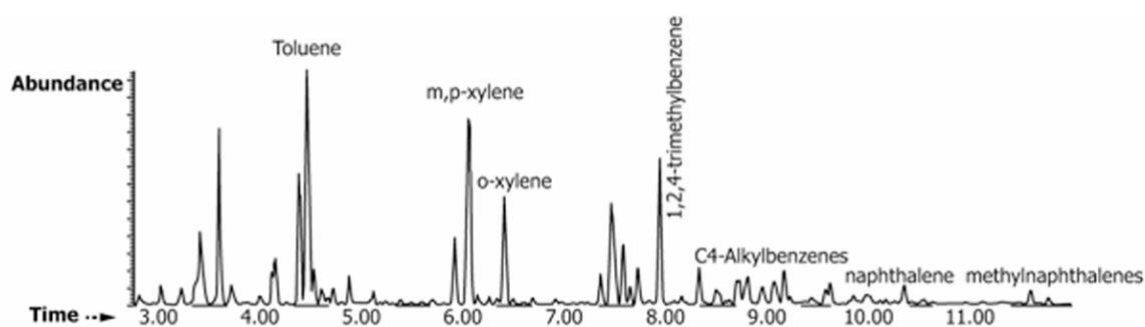


Figure 2.1: Example of a gasoline pattern; 50 % evaporated gasoline (ASTM E1618, 2019).

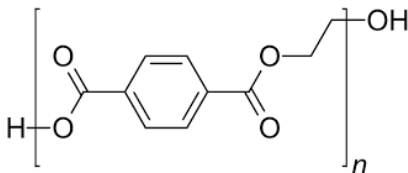
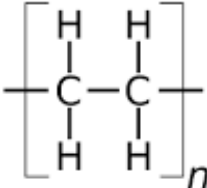
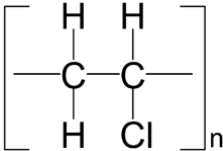
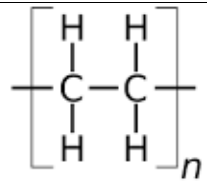
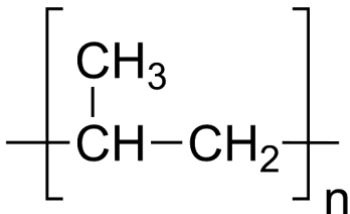
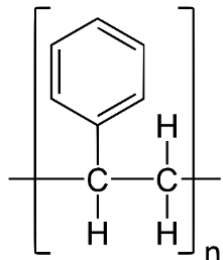
2.3 Plastics

Plastics are synthetic polymers and are considered as one of the most important inventions of the last century. They are widely used in daily life due to their versatility and ability to replace traditional materials such as metal, natural fiber, glass and wood. These macromolecules are also inexpensive to produce, possess favorable thermos-chemical properties and exhibit strong chemical resistance (Desidery & Lanotte, 2022). Moreover, plastics are convenient to use and offer various advantages, including being lightweight, durable, rust and water resistant, flexible, easily molded, suitable for mass production and excellent electrical insulators (Allen, 2025).

Structurally, plastics are mainly made of long-chain molecules called polymers, along with additives that modify or enhance material properties. Polymers are formed through polymerization, where small molecules called monomers join together step by step to form larger units like dimers, trimers and eventually high-molecular-weight chains. When a polymer is made from one type of monomer, it is known as a homopolymer, such as polyethylene. In contrast, polymers derived from two or more monomers are called copolymers, such as propylene-ethylene. The polymerization reaction is typically controlled through initiators or catalysts to regulate chain growth and molecular structure (Björkner et al., 2010).

The characteristics and properties of polymers depend on the nature, quantity and structural arrangement of their monomers, allowing their performance to be specifically tailored for targeted applications (Desidery & Lanotte, 2022). Plastics can be classified as thermoplastics, thermosets or elastomer. Thermoplastics are the most widely used because they can be melted and reshaped repeatedly, making them highly processable. In contrast, thermosets harden permanently once formed and are used when high strength or heat resistance is required. Meanwhile, elastomers are rubbery or elastic plastics that can be bent and stretched (Cantor & Watts, 2011; Wahab & Gund, 2024).

Table 2.4: Main polymer types, monomers, its chemical structure (Baheti, 2025).

Polymer Resin Identification Code	Polymers	Monomers
	Polyethylene Terephthalate	
	High-Density Polyethylene	 (lesser branching between polymer chains)
	Polyvinyl Chloride	
	Low-Density Polyethylene	 (excessive branching between polymer chains)
	Polypropylene	
	Polystyrene	
	Other plastics such as polycarbonate, acrylic, fibre, nylon	Different monomers are used for particular polymer

The general process of making plastic involves several steps: extraction, refining, polymerization and shaping. Raw materials such as petroleum and natural gas are extracted and then refined. During refining, crude oil is heated and distilled into different components, with naphtha being a key product used for plastic production as shown in Figure 2.2. In the polymerisation stage, gases are converted into polymers through either addition or condensation processes. Addition polymerisation links monomers into long chains, whereas condensation polymerisation bonds monomers while releasing water molecules. Finally, the polymers are mixed with additives and shaped it into the desired form (Asri, 2025).

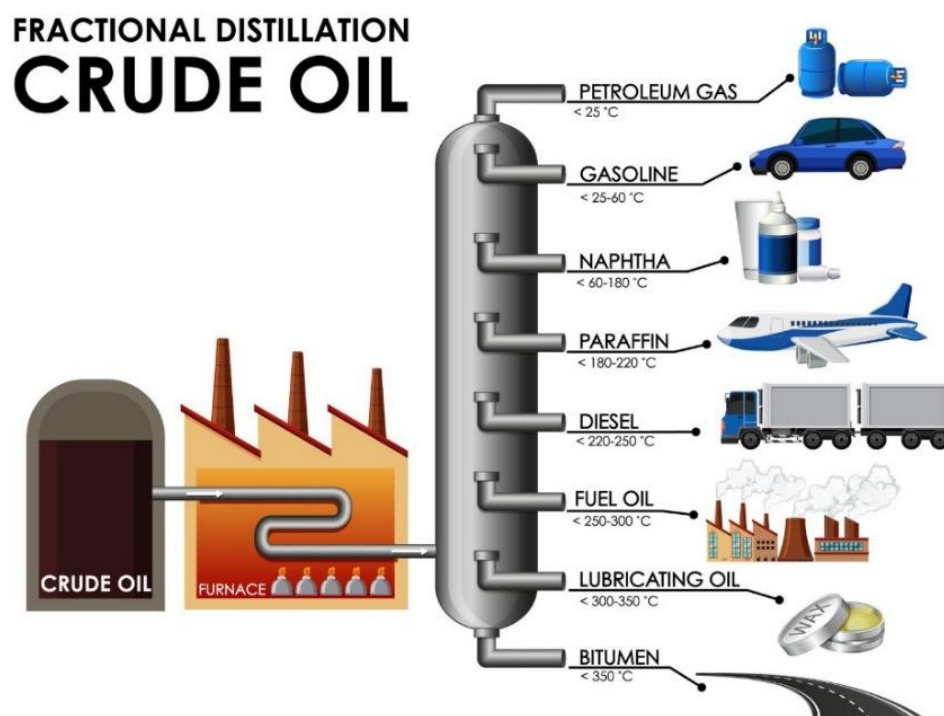


Figure 2.2: Fractional distillation of crude oil (Baheti, 2025).

2.3.1 Plastics in Fire Scenes

Within the last few decades, plastics have transformed the way we live. Although plastic existed earlier, the widespread production and use of plastics truly began in the 1950s and has continued to rise steadily ever since (Thompson et al., 2009). Today, plastics are used in almost every aspect of daily life, from the packaging of our favorite snacks to the electronic devices. Their versatility, durability and cost-effectiveness make them an essential material in the modern world (Median Kunststoff Service, 2024). Due to widely used of plastics, they are commonly found in residential, commercial and transportation environments. As a result, plastics are frequently present at fire scenes in the form of packaging materials, furniture components, electronic housings, vehicle interiors and many more.

When exposed to flame, many plastics significantly contribute to fire growth because they can melt, release flammable volatile compounds and act as an additional fuel source. The ease of ignition, rate of fire spread and overall fire behaviour depends greatly on the type of plastic involved (Devine et al., 2023). During heating, plastics experience thermal degradation. This process refers to the case where polymer chains of the plastic undergo chemical changes at elevated temperatures without the involvement of other reactants. This degradation can occur through main-chain scission, side-group rupture or cross-linking of polymers, which may result to the formation of volatile compounds and char residues (Pielichowski et al., 2022).

This thermal breakdown also known as pyrolysis. It involves decomposing complex polymer molecules into simpler ones using heat in the absence of oxygen. Pyrolysis generates a variety of products including bio-oil, syngas and char, as well as compounds such as aromatics, alkanes and alkenes. Different plastics have different pyrolysis behaviors and produce different degradation products depending on their chemical composition and molecular structure. For example, the pyrolysis of polyethylene (PE) and polypropylene (PP) at temperatures around 400-600°C yields high amounts of liquid products, whereas

polystyrene (PS) and polyvinyl chloride (PVC) produce mainly gaseous products. Plastics such as polyethylene terephthalate (PET) and polyurethane (PU) generate a mixture of liquid, gas and solid residues during pyrolysis (Lopez, 2023).

Many synthetic materials especially plastics are petrochemical-based and contain long hydrocarbon chains. When exposed to fire conditions, these materials undergo thermal degradation and pyrolysis, producing volatile and semi-volatile compounds (Chen et al., 2023) that fall within the same boiling-point range as commonly encountered ignitable liquids (ILs). Depending on the polymer type, plastics pyrolysis may generate compounds such as xylene, toluene and other volatile compounds that closely resemble ILRs (Jhaumeer-Laulloo et al., 2013). These conditions allow plastics to behave in an accelerant-like manner during the combustion due to the hydrocarbon chemistry and high energy content that can continuously feed the flame.

The contribution of pyrolysis products from solid substrates cannot be underestimated, as fire environments are chemically complex. During heating, plastics undergo side-group scission and other degradation mechanism that can create new carbon-based compounds which not originally present in the material. These newly formed products can overlap with characteristic ILs signatures, complicating the interpretation of fire debris (Zang et al., 2024). Among the various contributors to post-fire chemical complexity, substrate-derived residues are particularly challenging due to the wide variety of materials commonly present at fire scenes. As highlighted by NFPA 921 (2024), many plastic materials release hydrocarbon vapours during pyrolysis that can mimic petroleum-based accelerants.

2.4 Fourier Transform Infrared Spectroscopy (FTIR)

FTIR is an infrared spectroscopy analytical technique that widely used to identify and quantify molecular structures and functional groups by measuring the absorption of infrared (IR) radiation by a sample. IR occupies the region of the electromagnetic spectrum with frequencies ranging from 4 cm^{-1} to $140,000\text{ cm}^{-1}$, which situated between the microwave and visible light regions. Different regions of the electromagnetic spectrum are characterized by their radiation velocity and frequency, which is inversely proportional to wavelength (Yusuf, 2023). The IR region is divided into near-IR, mid-IR and far-IR ranges. Among these, the mid-IR region is most commonly employed in analytical applications, with the wavenumber range from 4000 cm^{-1} to 400 cm^{-1} (Fadlelmoula et al., 2022).

FTIR spectroscopy is extensively used for qualitative analysis, enabling the identification of functional groups and molecular structures in a wide range of materials. It can provide crucial information on the molecular structure of both inorganic and organic materials and is regarded as one of the most versatile non-destructive techniques for chemical characterization. Majority of compounds present in environment and industry are IR-active as molecules possessing a dipole moment are detectable by IR spectroscopy (Chen et al., 2015). In addition, FTIR can also be applied for quantitative analysis by determining the concentrations of components in the materials through the use of calibration models and chemometric approaches (Faturachman et al., 2025).

During FTIR analysis, absorption of IR radiation occurs when photons interact with molecules and promote them to higher vibrational energy states. These excited states correspond to various molecular vibrational modes, including stretching, twisting, bending, wagging, rocking and out-of-plane deformation, which occur at varying wavenumbers within the IR region. Each chemical bond or functional group absorbs IR radiation at characteristic wavenumbers, producing a distinctive spectral pattern. The intensity of these absorption bands is directly related to the abundance of the corresponding functional groups and is

measured using either the maximum peak height or the integrated peak area relative to a defined baseline (Chen et al., 2015).

FTIR spectroscopy employs a mathematical Fourier Transform to convert the raw interferogram, which contains mixed-frequency signals into a conventional IR spectrum plotted as intensity versus wavenumber. Several sampling techniques are available in FTIR analysis, including transmission and reflection methods. The transmission method is one of the simplest, most widely used approach and suitable for the analysis of gases, liquids and solids samples (Yusuf, 2023). FTIR spectra may be displayed either as transmittance versus wavenumber or absorbance versus wavenumber. Both representations contain the same information and differ only by mathematical inversion. Although many spectral libraries and interpretation guides are presented in absorbance format, transmittance spectra can be readily converted when required.

A typical mid-IR FTIR spectrum (4000 to 400 cm^{-1}) is commonly divided into two principal interpretation regions which are the functional group region and the fingerprint region. Each of these regions providing distinct analytical information. More specifically, the mid-IR spectrum can be subdivided into four regions which are the single-bond region (4000–2500 cm^{-1}), the triple-bond region (2500–2000 cm^{-1}), the double-bond region (2000–1500 cm^{-1}) and the fingerprint region (1500–600 cm^{-1}) (Nandiyanto et al., 2019), as shown in the Figure 2.3. The fingerprint region contains a complex pattern of absorption bands that is highly specific to individual compounds. This region is valuable for distinguishing molecules with similar functional groups, differentiating polymers with identical repeat units but varying structural arrangements and enabling detailed characterization of complex materials and natural products (Ramírez-Hernández et al., 2019; Dev & Mukadam, 2025).

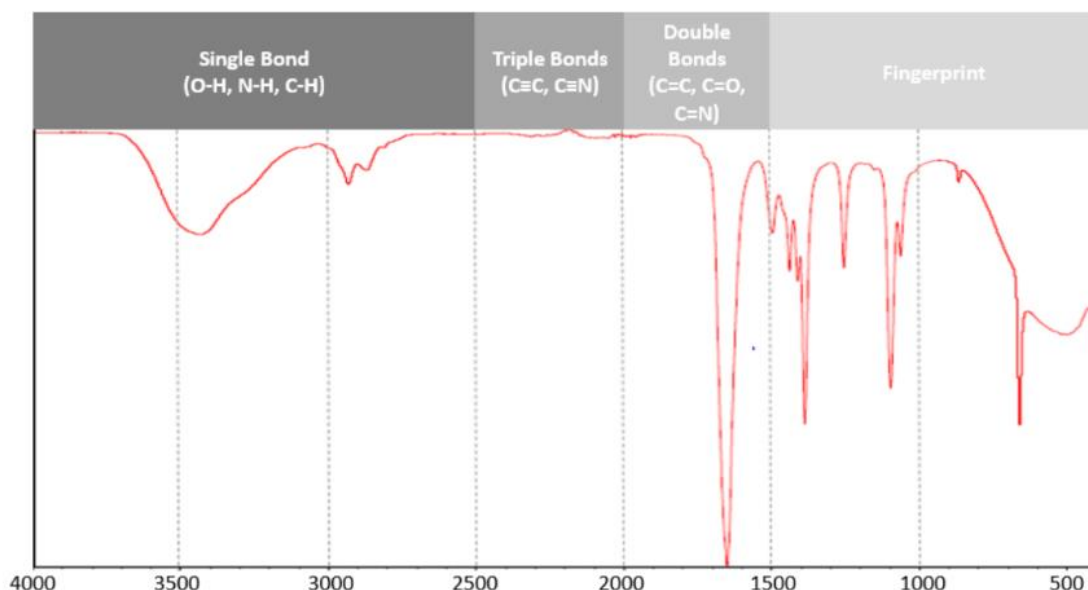


Figure 2.3: Mid-IR spectrum region (Nandiyanto et al., 2019).

2.4.1 FTIR Analysis of Plastic Products

Plastics are organic polymers composed of functional groups such as C–H, C–C, C=O, C–O, C–Cl and N–H. These chemical bonds are IR-active due to changes in dipole moment during vibration and therefore generate strong and well-defined absorption bands in IR spectra (Nandiyanto et al., 2023; Hsiao et al., 2025). As a result, FTIR spectroscopy can be used for the characterization of plastic, as it provides essential chemical and structural information. The technique enables the identification of polymer types, additives and degradation products through the detection of characteristic vibrational transitions associated with specific functional groups. By measuring the absorption of IR radiation, FTIR produces a distinctive spectral profile commonly described as a molecular fingerprint. This spectral can be compared with reference spectral libraries for reliable material identification (Fonkou et al., 2025).

FTIR spectroscopy has been widely applied to characterize common plastic materials in both consumer and environmental contexts. There is a recent open-access dataset reported by Villegas-Camacho et al. (2024), which covers FTIR spectra of six major industrial plastic polymers which are Polyethylene Terephthalate (PET), High-Density Polyethylene (HDPE),

Polyvinyl Chloride (PVC), Low-Density Polyethylene (LDPE), Polypropylene (PP) and Polystyrene (PS). In this dataset, spectral data are presented in transmittance percentage as the “y” variable and wavenumber (cm^{-1}) as the “x” variable. Transmittance is used as it directly reflects the proportion of IR radiation passing through the sample and can offer a more intuitive information of the vibrational behavior of molecular bonds in polymers compared to absorbance. Usually, absorbance values often require additional interpretation to fully relate the spectral intensity to the extent of molecular vibration.

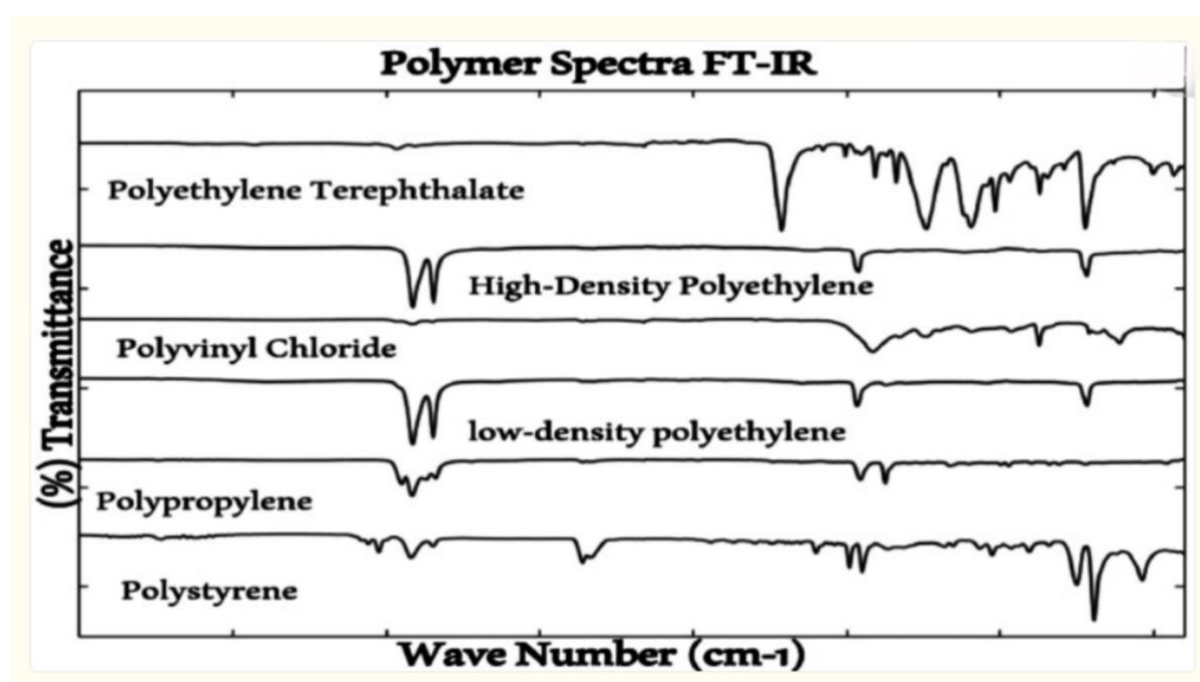


Figure 2.4: Example of the FTIR spectra of the six most used industrial plastics (Villegas-Camacho et al., 2024)

PET exhibits characteristic absorption bands associated with ester functional groups and aromatic ring structures. A strong absorption band in the region of $1730\text{--}1710\text{ cm}^{-1}$ can be observed, corresponding to the $\text{C}=\text{O}$ stretching vibration of the ester linkage. In the region between $1600\text{--}1500\text{ cm}^{-1}$, the absorption bands are attributed to $\text{C}=\text{C}$ stretching vibrations of the aromatic ring. Additionally, bands observed in the region of $1250\text{--}1100\text{ cm}^{-1}$ are assigned to $\text{C}\text{--}\text{O}\text{--}\text{C}$ stretching vibrations of the ester group (Dodi et al., 2022; Avadanei et al., 2024).

HDPE and LDPE are chemically similar polyolefins composed of repeating ($-\text{CH}_2-$) units. Both polymers display strong absorption bands near 2915 and 2848 cm^{-1} , corresponding to asymmetric and symmetric C–H stretching vibrations, respectively. The absorption bands around 1470 – 1460 cm^{-1} arise from CH_2 bending vibrations and the bands observed in the region of 1377 – 1368 cm^{-1} are associated with CH_3 bending vibrations originating from the chain ends or branching. The bands in the region of 1377 – 1368 cm^{-1} are typically more intense in branched LDPE than in HDPE. Thus, it can be used to distinguish between the two polyethylene (PE) types (Da Silva & Wiebeck, 2022).

PVC possesses a simple ($-\text{CH}_2-\text{CHCl}-$) backbone, producing FTIR spectrum that is dominated by C–Cl and C–H vibrations modes. The presence of chlorine atoms in the polymer backbone give rise to distinctive absorption features in the low-wavenumber region, particularly between approximately 835 – 830 cm^{-1} and 690 – 615 cm^{-1} , which are attributed to C–Cl stretching vibrations. In addition, C–H stretching vibrations are observed in the region of 3000 – 2800 cm^{-1} . The bands associated with CH_2 and $\text{CH}-\text{Cl}$ bending and deformation modes may also be observed in the region between 1430 – 1250 cm^{-1} (Abdelghany et al., 2019).

PP is a saturated polyolefin containing both CH_3 and CH_2 groups, which may result in a more complex C–H stretching and bending region compared to PE. Characteristic absorption bands are observed in the region of 2950 – 2835 cm^{-1} , corresponding to asymmetric and symmetric aliphatic C–H stretching vibrations. Additionally, bending vibrations of CH_3 groups can be observed near the 1455 and 1375 cm^{-1} . The presence of prominent methyl bending bands allows differentiation of PP from PE, which lacks significant CH_3 vibrations due to the absence of methyl groups in its polymer backbone (Curcic et al., 2025).

PS consists of an aliphatic $-\text{CH}_2-\text{CH}(\text{Ph})-$ backbone with a monosubstituted benzene ring. This polymer is identified by its aromatic ring structure, with aromatic C–H stretching vibrations observed in the region of $3080\text{--}3025\text{ cm}^{-1}$. In addition, the absorption bands corresponding to aromatic C=C stretching vibrations are observed between $1600\text{--}1450\text{ cm}^{-1}$. The bending vibrations of aromatic ring and C–H bonds can be seen in the region of $1490\text{--}1450\text{ cm}^{-1}$. Moreover, the observed bands near $760\text{--}700\text{ cm}^{-1}$ are attributed to out-of-plane C–H bending vibrations of the benzene ring (Muhemmed & Aziz, 2025).

Polycarbonate (PC) consist of repeating carbonate linkage ($-\text{O}-\text{CO}-\text{O}-$) connecting aromatic bisphenol A units. This polymer is identified by a strong absorption band in the region of $1770\text{--}1765\text{ cm}^{-1}$, corresponding to the stretching vibration of C=O group. In addition, aromatic C=C stretching vibrations from the phenyl rings are observed between $1600\text{--}1500\text{ cm}^{-1}$, together with bands in the region of $1220\text{--}1060\text{ cm}^{-1}$ attributed to C–O–C stretching vibrations of carbonate linkage (Nandiyanto et al., 2023).

Polyurethane (PU) consist of repeating urethane linkages ($-\text{NH}-\text{CO}-\text{O}-$). This polymer is identified by the presence of C=O stretching vibration of the urethane group in the region of $1730\text{--}1700\text{ cm}^{-1}$. Moreover, N–H stretching vibrations can be observed in the region around $3335\text{--}3200\text{ cm}^{-1}$, while N–H bending (amide II) vibrations observed near $1540\text{--}1520\text{ cm}^{-1}$. In the region of $1250\text{--}1050\text{ cm}^{-1}$, the bands observed are associated with C–O–C stretching vibrations of urethane linkage, while aliphatic C–H stretching vibrations are observed between $2950\text{--}2850\text{ cm}^{-1}$ (Delpech & Miranda, 2011).

Butyl rubber (IIR) consists of saturated hydrocarbon backbone formed from isobutylene units with small proportion of isoprene segments. This elastomer is identified by strong aliphatic C–H stretching vibrations observed in the region of $2950\text{--}2850\text{ cm}^{-1}$. In addition, a weak absorption band corresponding to C=C stretching vibrations from residual

isoprene is observed near 1660–1600 cm^{-1} , while the bending vibrations of CH_2 appear in the region of 1450–1375 cm^{-1} . The bands observed below 1000 cm^{-1} are attributed to skeletal vibrations of the rubber backbone (Smith, 2022).

2.5 Chemometric Analysis

Chemometrics is a multidisciplinary field that applies mathematical and statistical methods to extract relevant information from chemical data. The increased in computational power has enabled the widespread use of chemometrics for processing large and complex datasets generated by advanced analytical instruments within a short time (Zappi et al., 2023). These techniques are widely employed in modern chromatographic and spectrometric methods. Chemometrics approaches are applied in analytical protocol development, multivariate data analysis, process modelling, calibration, prediction, pattern recognition, classification, data reduction, graphical visualization and statistical process control (Singh et al., 2023).

Chemometrics techniques can be broadly classified into unsupervised and supervised methods. Unsupervised methods are exploratory techniques that analyze data without prior information of sample classes or group labels to reveal inherent patterns, similarities and differences within a dataset based solely on the measured variables. Commonly used unsupervised techniques include Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA). In contrast, supervised methods utilise prior knowledge of known class membership to develop models for the classification and prediction of future samples, enabling more targeted and reliable analytical interpretation (Santos et al., 2013). Commonly used supervised techniques include Linear Discriminant Analysis (LDA) and Soft Independent Modelling of Class Analogy (SIMCA).