

Determination of Persistence of Accelerant in Household Materials Using Atr-Ftir Spectroscopy

Devika M Reji¹, Aiswaria R²

¹Post Graduate MSC Forensic Science, MES Kalladi College Mannarkkad, Palakkad, Kerala, India

²Assistant Professor, Department of forensic science, MES Kalladi College Mannarkkad, Palakkad, Kerala, India

Abstract

This study investigates the persistence of accelerants in fire debris from common household materials—paper, cloth, rubber, carpet, and wood—using Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy (ATR-FTIR). These materials, prevalent in typical home environments, were cut into standardized pieces and ignited with petrol, a common arson accelerant. The resulting fire debris was collected and analyzed at predetermined intervals to detect and measure petrol residues using ATR-FTIR, which identifies distinctive absorption peaks associated with the accelerant. The findings revealed a progressive decline in the detectable presence of petrol across all materials over time. However, the rate at which petrol residues diminished varied significantly among the different materials. Some materials retained detectable levels of accelerant longer than others, highlighting the influence of material composition on accelerant persistence. This variability underscores the importance of material type in forensic analyses of fire debris, as it affects the duration and detectability of accelerant residues. These insights are crucial for forensic investigations, improving the accuracy of determining the presence and quantity of accelerants used in suspected arson cases. Understanding how different materials interact with accelerants over time allows forensic scientists to better reconstruct fire events and identify the cause of fire. The study demonstrates that ATR-FTIR is a reliable method for detecting and analyzing accelerant residues, enhancing the capability of forensic professionals to investigate and solve arson cases. Overall, this research contributes valuable knowledge to forensic science by detailing how accelerant residues persist in various household materials after a fire

Keywords: ATR-FTIR, Fire debris, Paper, Wood, Cloth, Carpet, Rubber, Petrol

INTRODUCTION

Fire is a remarkable phenomenon that has played a crucial role in human evolution, enabling advancements such as cooking, warmth, and protection. Even today, fire remains essential for various functions, including energy production and illumination. However, it also poses significant risks if not managed properly, emphasizing the need for safety precautions (Smith, 2018).

Fire consists of chaotic flames, each with a thickness of approximately 10^{-3} to 10^{-2} cm, producing energy at around 10^8 to 10^9 W/cm³ (Jones & Patel, 2020). Flames can arise through premixed combustion, where reactants are mixed before ignition, or diffusion flames, where mixing occurs during combustion. In both cases, the reaction occurs in the gas phase, generating the characteristic flame structure. Generally, fire represents an exothermic reaction, often triggered by temperature increases or

catalytic activity, leading to a self-sustaining combustion process (Brown et al., 2017).

Arson is a serious crime that endangers lives and property, often motivated by factors such as financial gain, revenge, or psychological distress. While some argue that arson should be treated as a mental health issue, it remains a criminal offense with severe legal consequences. Investigators rely on forensic techniques, including accelerant detection and fire pattern analysis, to determine the cause of suspicious fires (Yadav et al., 2020; Banyal, 2023)

Accelerants are flammable substances, often liquids like gasoline, kerosene, and alcohol, intentionally used to accelerate fire spread and intensity in arson cases. These materials make fires more destructive and difficult to control, endangering lives and property. Arson investigators detect accelerants using fire pattern analysis and forensic testing of debris samples, identifying chemical residues that indicate intentional ignition (Banyal, 2023; Yadav et al., 2020).

Gasoline, or petrol, is a petroleum-derived liquid used in combustion engines, consisting of hydrocarbons and additives like oxygenates and antioxidants. It has a low flash point (-43°C) and high flammability, making it significant in forensic investigations of arson and fuel-related crimes. Gasoline combustion releases pollutants, including carbon monoxide, nitrogen oxides, and greenhouse gases, contributing to air pollution and climate change (Yadav et al., 2020).

Arson investigation relies on understanding the fire triangle—fuel, oxygen, and heat—along with fire dynamics and building construction to determine fire origin and cause. Investigators analyze fire patterns, collect forensic evidence, and use instrumental techniques to detect accelerants. Key methods include Gas Chromatography-Mass Spectrometry (GC-MS) and Fourier Transform Infrared Spectroscopy (FTIR) to identify ignitable liquid residues. Proper sampling, especially from porous materials like carpets and wood seams, is crucial for retaining volatile residues. Challenges such as pyrolysis products, weathering, and bacterial degradation complicate forensic analysis (Banyal, 2023; Yadav et al., 2020).

Fourier-transform infrared spectroscopy (FTIR) is a widely used technique for analyzing the chemical composition and molecular structure of materials like polymers. It measures infrared light absorption across different wavelengths, revealing functional groups, detecting impurities, and providing molecular insights. The mid-IR region ($4000\text{--}400\text{ cm}^{-1}$) is particularly useful for identification. ATR-FTIR, a leading sampling technique, enables rapid analysis with minimal preparation by using total internal reflection, enhancing sensitivity and specificity. The evanescent wave penetration depends on the refractive index difference between the sample and the ATR crystal, making it adaptable for various sample types

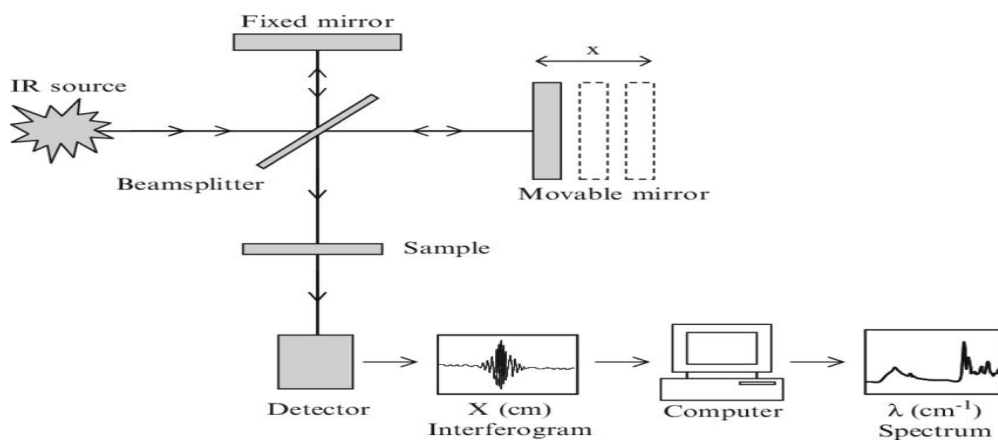


Fig 1. Schematic representation of infra-red spectroscopy¹

FTIR is a non-destructive and reliable analytical method used to identify unknown chemical compositions in various materials, including polymers, organic, and some inorganic substances. In forensic investigations, it aids in detecting chemicals from paints, fire debris, synthetic materials, polymer coatings, drugs, and accelerants. While GC-MS is commonly used for accelerant detection, fewer studies have applied FTIR for this purpose. This study aims to assess petrol persistence in household materials by analyzing fire debris samples using FTIR, providing insights into its role in household fires and safety concerns.

CASE STUDIES

The **Himachal Pradesh forest sales depot fire** was initially reported as an electrical short-circuit but was later confirmed as arson due to multiple ignition points and forensic evidence contradicting official claims. In **Chicago**, a wrongful arson conviction led to a death sentence, but later scientific investigations revealed flaws in the original findings, resulting in a pardon. A **duplex fire** investigation linked a woman to the crime through gasoline traces, fingerprints, and witness testimonies, leading to her institutionalization. A **plastics manufacturing fire** showed multiple ignition points and forced entry, with the owner's possession of oil-stained shoes and matching tools confirming his guilt. In a **convenience store fire**, missing inventory, forced entry, and CCTV footage placed the financially troubled owner at the scene, resulting in an arson charge. **Gary L. DeTemple** committed multiple arsons for insurance fraud, leading to his conviction and imprisonment. **The Future Now, Inc. arson** was part of a multi-million-dollar theft and fire scheme, resulting in multiple arrests and convictions. The **2002 Godhra train burning**, allegedly carried out by a mob, led to multiple convictions but remains a controversial event in India's history. The **Best Bakery case**, linked to the Gujarat riots, initially resulted in acquittals due to weak evidence, but a Supreme Court-ordered retrial led to several convictions, though some were later overturned or reduced.

Aim

To determine the persistence of accelerant in fire debris of various household materials using ATR- FTIR.

Objectives

1. To determine the persistence of accelerant in the burned residue of various household materials
2. To identify the variation in the persistence of accelerant in various household materials- depending on time

MATERIALS AND METHODS

SAMPLE COLLECTION:

Most common household materials such as paper, cloth, rubber, carpet, and wood were cut into pieces measuring 10cm in length, 5cm in breadth, and 2cm in height. Five samples of each material were collected for testing.

MATERIAL REQUIREDThe required materials include paper, rubber, cloth, wood, and carpet to test accelerant retention, along with scissors, a measuring cup, and a scale for precise sample preparation. Petrol is used as the accelerant due to its volatility and forensic relevance. A matchbox ignites samples, while tweezers handle debris safely. A metal can ensures controlled burning, and a marker labels samples for tracking. These materials support analyzing petrol's persistence on various substrates using ATR-FTIR.

Instrument required

FTIR (Fourier Transform Infrared Spectroscopy) is an analytical instrument used to identify chemical co-

mpounds based on their molecular vibrations. It detects functional groups in a sample by measuring the absorption of infrared light, providing a unique spectral fingerprint. In this study, ATR-FTIR (Attenuated Total Reflectance FTIR) allows for non-destructive analysis of fire debris, helping to detect and confirm the presence of petrol residues on different materials post-combustion.

METHODOLOGY:

The experiment was conducted in a controlled indoor environment at room temperature. We measured household materials using a scale with a precision of 10 cm in length, 5 cm in breadth, and 2 cm in height. Approximately 15 ml of petrol was accurately measured and added to the samples in a measuring jar. Five distinct samples were ignited and observed as they burned partially. After each sample burned, it was carefully collected in a labelled metal can using tweezers at specific time intervals for further analysis.



Fig 2: Burned fire debris

After initializing the FTIR instrument, the sample holder was cleaned with acetone and tissue. The transmittance spectrum range was set from 400 to 4000 cm^{-1} , with 45 scans per measurement and a resolution of 4. A background scan was conducted before each burned sample was sequentially measured. The sample holder was cleaned between samples to prevent cross-contamination.



Fig 3: ATR-FTIR

Transmittance spectra ranging from 400 to 4000 cm^{-1} were obtained for each burned sample using the FTIR instrument. These spectra were subsequently converted to absorbance spectra using Microsoft Excel. The spectral data were then analyzed and compared using Lab Solution IR Software and Origin

Pro software.

Table 1 Variation in persistence of accelerant

SAMPLES	TIME INTERVALS				
	15 MINUTES	30 MINUTES	1 HOUR	1 HOUR 30 MINUTES	2 HOURS
CLOTH	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	×	×
RUBBER	<input type="checkbox"/>	<input type="checkbox"/>	×	×	×
WOOD	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	×	×
PLASTIC CARPET	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	×	×
PAPER	<input type="checkbox"/>	<input type="checkbox"/>	×	×	×

The mentioned Table 1 appears that the materials which have the presence of accelerants as the passage of time. The determination slowly diminish as the time moves on.

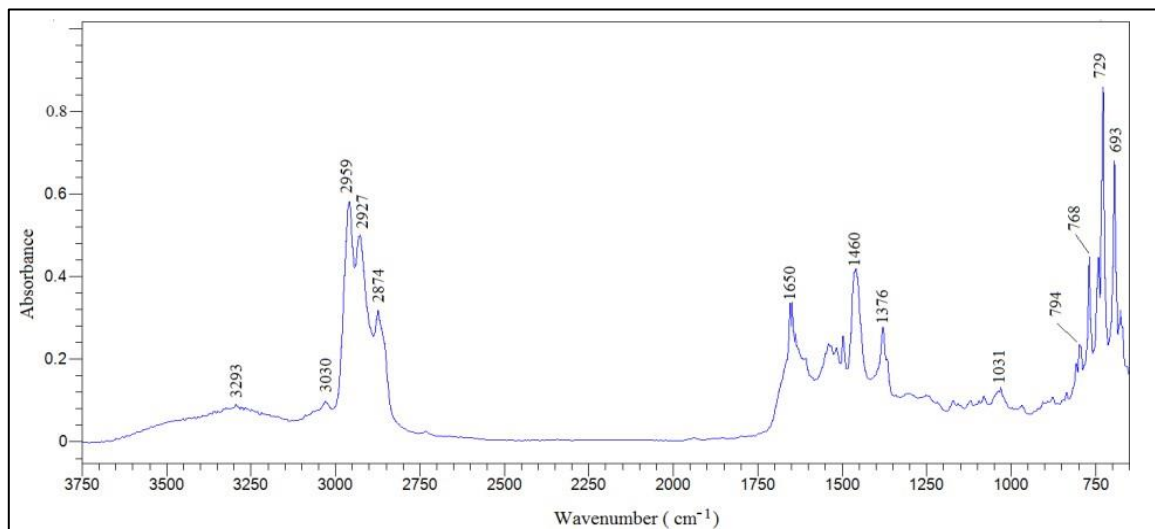
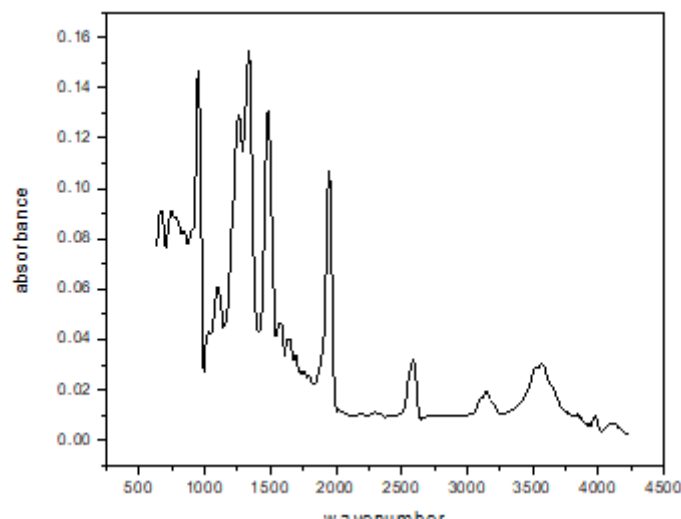
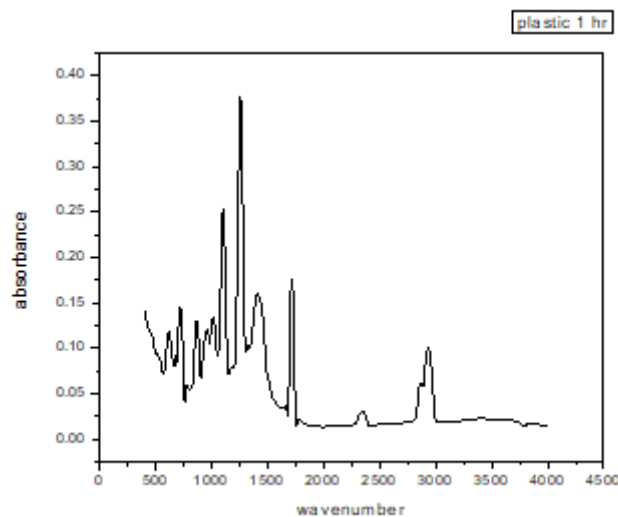
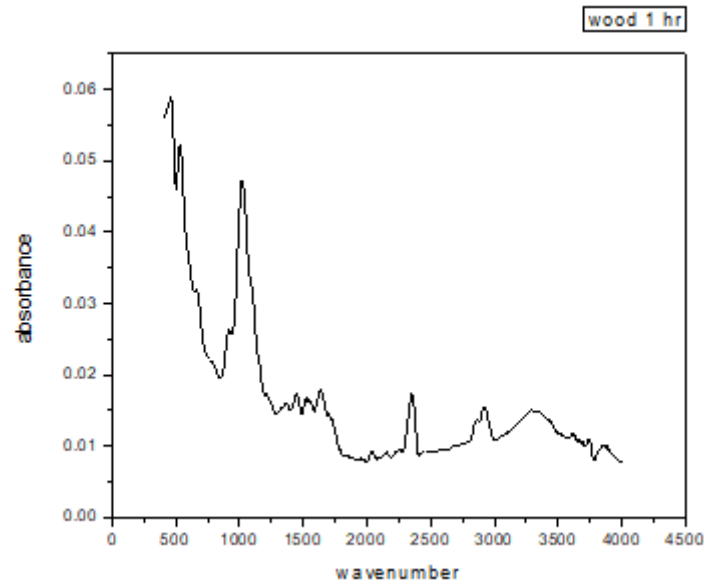


Fig 4. FTIR-ATR spectrum of gasoline (MS quality) in the 650-3750 cm⁻¹ region

Figure 4 presents the standard FTIR-ATR spectrum of gasoline, highlighting the peaks corresponding to the C-H stretching vibrations of alkanes, the O-H stretching vibrations of the hydroxyl functional group, and the C-H stretching vibrations of aromatic compounds





DISCUSSION

A total of 25 samples were subjected to combustion after the introduction of petrol, and they were gathered at various time intervals throughout the process. Subsequently, the burned residues of these samples were subjected to analysis using ATR-FTIR (Fourier-transform infrared spectroscopy). The resulting spectra obtained from the analysis were then compared with the standard spectrum of petrol to accurately identify the specific peaks present in the samples.

Petroleum is a complex mixture of hydrocarbons and heteroatomic compounds. The main classes of compounds found in petroleum are alkanes, which are straight or branched chain saturated hydrocarbons, cycloalkanes, which are saturated hydrocarbons with one or more carbon rings, aromatics, which are unsaturated hydrocarbons containing one or more benzene rings, and heteroatomic compounds, which contain nitrogen, sulfur, and/or oxygen atoms in addition to carbon and hydrogen. These compounds make up the wide range of molecules found in petroleum, each with its own unique chemical and physical properties. Major peaks found in the standard petrol spectrum range from 600-3750 cm^{-1} region. The strong bands in the 3000-2750 cm^{-1} region are caused by the CH stretching vibrations of alkanes. The IR

absorption peaks observed in the 1300-1700 cm^{-1} region are mainly due to C=C and CH (scissoring) of the skeletal modes. Peaks below 1000 cm^{-1} are mostly caused by out-of-plane vibrations in aromatic and other cyclic hydrocarbons.

The study highlights the significant role of time and material properties in the persistence of accelerant residues in fire investigations. ATR-FTIR analysis revealed that absorption peaks corresponding to petrol decrease over time, with porous materials such as cloth, wood, and plastic retaining residues for up to an hour. This suggests that these materials can serve as crucial forensic evidence post-fire.

The findings also indicate that some materials develop a charred outer layer that insulates the inner layers, limiting combustion and preserving accelerant traces. This effect is particularly relevant in forensic analysis, as it can help identify accelerants even after exposure to fire. However, the volatile nature of accelerants necessitates timely sample collection to maximize detection accuracy.

While ATR-FTIR is a valuable tool for identifying fire residues, it has limitations, such as interference from overlapping absorption bands and surface sensitivity, which may lead to incomplete data. Future research could expand on these findings by analyzing a broader range of materials and incorporating complementary analytical techniques. This study underscores the importance of understanding material behavior in fire investigations and highlights the need for prompt forensic analysis to ensure the reliable detection of accelerant residues.

Conclusions

The study investigated the effect of time and the nature of materials on the persistence of accelerants over extended periods. Five different household materials—cloth, plastic, carpet, wood, and another unspecified material—were selected for this experiment. Each material was soaked with petrol and then burned to simulate fire conditions.

Residue samples were collected at various time intervals post-burning to assess how long the accelerant persisted on each material. These samples were analysed using ATR-FTIR (Attenuated Total Reflectance Fourier-Transform Infrared Spectroscopy), which provides detailed chemical analysis by generating absorption spectra.

The absorption spectra produced by ATR-FTIR during the analysis were compared with standard spectra of known accelerants to identify and quantify the presence of residual accelerants in the samples.

The results revealed that the persistence of accelerants is significantly influenced by both the elapsed time since the fire and the type of material involved. Specifically, materials such as cloth, plastic, carpet, and wood showed a notable capacity to retain accelerants for longer periods, effectively preventing their rapid evaporation. This finding underscores the importance of considering both time and material type in forensic investigations of fire scenes, as these factors can critically impact the detection and analysis of accelerants in fire debris.

REFERENCES

1. Alien, D., Petrakis, L., Grandy, D., Gavalas, G., & Gates, B. (1984). Determination of functional groups of coal-derived liquids by n.m.r. and elemental analysis. *Fuel*, 63(6), 803–809. [https://doi.org/10.1016/0016-2361\(84\)90071-1](https://doi.org/10.1016/0016-2361(84)90071-1)
2. Almirall JR and Furtpn KG (eds) Analysis and interpretation of fire scene evidence. Boca Raton: CRC Press, 2004
3. Almirall, Jose R., and Kenneth G. Furton. Analysis and interpretation of fire scene evidence. CRC pr-

sess, 2004.

4. American Society for Testing and Materials. (n.d.-b). Accelerants. https://www.salempress.com/Media/SalemPress/samples/forensic_pgs.pdf
5. Andrew.Davies. (2023, March 14). Attenuated Total Reflectance ATR-FTIR Spectroscopy Principles. Specac Ltd. <https://specac.com/theory-articles/introduction-to-atr-ftir->
6. Daeid, N. N. (2015). Chemistry of Fire. Forensic Chemistry, 201.
7. 'Daly, S. R., Niemeyer, K. E., Cannella, W. J., & Hagen, C. L. (2016). Predicting fuel research octane number using Fourier-transform infrared absorption spectra of neat hydrocarbons. Fuel, 183, 359–365. <https://doi.org/10.1016/j.fuel.2016.06.097>
8. Daly, S. R., Niemeyer, K. E., Cannella, W. J., & Hagen, C. L. (2016b). Predicting fuel research octane number using Fourier-transform infrared absorption spectra of neat hydrocarbons. Fuel, 183, 359–365. <https://doi.org/10.1016/j.fuel.2016.06.097>
9. Dembsey, N. A. (2007). Review of “Fundamentals of Fire Phenomena” by James G.
10. Frontela, L., Pozas, J. A., & Picabea, L. (1995). A comparison of extraction and adsorption methods for the recovery of accelerants from arson debris. Forensic science international, 75(1), 11-23.
11. Gremlich, H. (2000). Infrared and raman spectroscopy. Ullmann’s Encyclopedia of Industrial Chemistry. https://doi.org/10.1002/14356007.b05_429
12. Griffiths, P. R., & De Haseth, J. A. (2006c). Fourier Transform Infrared Spectrometry. <https://doi.org/10.1002/047010631x>
13. Gurvinder Singh Bumbrah, Rajinder Kumar Sarin, Rakesh Mohan Sharma (2016) Derivative Ultraviolet Spectrophotometry: A Rapid, Screening Tool for the Detection of Petroleum Products Residues in Fire Debris Samples.
14. Guzmán-Osorio, F., Domínguez-Rodríguez, V., Adams, R., Lobato-García, C., Guerrero- Peña, A., & Barajas-Hernández, J. (2021). Classification of petroleum origin and integrity by FTIR. Egyptian Journal of Petroleum/Egyptian Journal of Petroleum, 30(2), 63–67. <https://doi.org/10.1016/j.ejpe.2021.03.003>
15. harma, K. (2023, July 8). FTIR : Principle, instrumentation, applications, advantages,.Science Info.<https://scienceinfo.com/ftir-principle-instrumentation- applications/#limitations-of-ftir>
16. iegel JA, Knupfer GC and Saukko PJ. Encyclopedia of forensic sciences. Vol. 1–3. 1st ed. London: Academic Press, 2000.
17. Kerr, T. J., Duncan, K. L., & Myers, L. (2013). Application of vibrational spectroscopy techniques for material identification from fire debris. Vibrational Spectroscopy, 68, 225–235. <https://doi.org/10.1016/j.vibspec.2013.08.006>
18. Khanmohammadi, M., Garmarudi, A. B., Garmarudi, A. B., & De La Guardia, M. (2012). Characterization of petroleum-based products by infrared spectroscopy and chemometrics. TrAC. Trends in Analytical Chemistry, 35, 135–149. <https://doi.org/10.1016/j.trac.2011.12.006>
19. Lalnunthari, J., & Thanga, H. H. (2015). Detection of Methyl tert-butyl Ether (MTBE) in Gasoline Fuel using FTIR: ATR spectroscopy. International Research Journal of Environmental, 4(12), 65-68.
20. Lalramnghaka, J., Thanga, H. H., & Biaktluanga, L. (2023). Evaluation of gasoline fuel quality using FTIR spectroscopy and multivariate technique: a case study in Aizawl city. Petroleum Science and Technology, 41(6), 677-699.

21. Marshall, A. G., & Rodgers, R. P. (2008). *Petroleomics: Chemistry of the underworld*. Proceedings of the National Academy of Sciences of the United States of America, 105(47), 18090–18095. <https://doi.org/10.1073/pnas.0805069105>
22. Martina, M., Halmer. (2006). Limitations of FTIR Spectroscopy for Detection of Water in Spinel Group Minerals, When $IVFe^{2+}$ is Incorporated into the Crystal Structure. *Spectroscopy Letters*, 39(2):181-186. doi: 10.1080/00387010500531217
23. Martín-Alberca, C., Ortega-Ojeda, F. E., & García-Ruiz, C. (2016). Analytical tools for the analysis of fire debris. A review: 2008–2015. *Analytica Chimica Acta*, 928, 1-19.
24. Ojeda, J. J., & Dittrich, M. (2012). Fourier transform infrared spectroscopy for molecular analysis of microbial cells. *Microbial Systems Biology: Methods and Protocols*, 187-211.
25. Pavoni, B., Rado, N., Piazza, R., & Frignani, S. (2004). FT-IR Spectroscopy and Chemometrics as a useful approach for determining Chemical-Physical properties of gasoline, by minimizing analytical times and sample handling. *Annali Di Chimica*, 94(7– 8), 521–532. <https://doi.org/10.1002/adic.200490066>
26. Perkins, W. D. (1986). Topics in Chemical Instrumentation: Fourier Transform-Infrared Spectroscopy: Part I. Instrumentation. *Journal of Chemical Education*, 63(1). <https://eric.ed.gov/?id=EJ333564>
27. Pert, A. D., Baron, M. G., & Birkett, J. W. (2006). Review of analytical techniques for arson residues. *Journal of forensic sciences*, 51(5), 1033-1049.
28. Petit, S., & Madejova, J. (2013). Fourier Transform Infrared Spectroscopy. In *Developments in clay science* (pp. 213–231). <https://doi.org/10.1016/b978-0-08-098259-5.00009-3>
29. Quintiere, Wiley, 2006, ISBN-13 978-0-470-09113-5 and ISBN-10 0-470-09113-4. *Fire*
30. Richard Tuve & Dawson Powell. (n.d.). *Fire Arson Investigation Manual Chemistry and Physics of Fire Behaviour*. In *Principles of Fire Protection Chemistry*. <http://courseware.cutm.ac.in/wp-content/uploads/2020/07/Fire-Arson-Investigation-Manual-2002.pdf>
31. Sandercock, P. M. L. (2008). Fire investigation and ignitable liquid residue analysis—a review: 2001–2007. *Forensic science international*, 176(2-3), 93-110.
32. Sandercock PML. Fire investigation and ignitable liquid residue analysis – a review: 2001–2007. *Forensic Sci Int* 2006; 176: 93–110.
33. Schobert, H. (2013b). Composition, classification, and properties of petroleum. In *Cambridge University Press eBooks* (pp. 174–191). <https://doi.org/10.1017/cbo9780511844188.012>
34. Skoog DA, Holler FJ and Crouch SR. *Principles of instrumental analysis*. Boston: Cengage Learning, 2006
35. Smith B.C., *Infrared Spectral Interpretation: A Systematic Approach*, CRC Press, 78 (1999)
 - i. [spectroscopy-part-1-the-basics/](#)
36. Speitel, L. C. (2002). Fourier Transform Infrared Analysis of combustion gases. *Journal of Fire Sciences*, 20(5), 349–371. <https://doi.org/10.1177/0734904102020005484>
37. Stach, R., & Mizaikoff, B. (2017). Fuel Performance Specifications, Mid-Infrared Analysis of. *Encyclopedia of Analytical Chemistry*, 1–16. <https://doi.org/10.1002/9780470027318.a1810.pub2>
38. Stauffer E, Lentini J. ASTM methods for fire debris analysis: a review. *Forensic Sci Int* 2003; 132:63–7.
39. Stauffer, E., & NicDaéid, N. (2013). Chemistry of fire. In *Elsevier eBooks* (pp. 161–166). <https://doi.org/10.1016/b978-0-12-382165-2.00098-2>
40. Stauffer, E., Dolan, J. A., & Newman, R. (2007). *Fire debris analysis*. Academic Press.

41. Swarin, S. J., & Drumm, C. A. (1991). Prediction of Gasoline Properties with NearInfrared Spectroscopy and Chemometrics. SAE Technical Papers on CD-ROM/SAE Technical Paper Series. <https://doi.org/10.4271/912390>
42. Technology, 43(1), 91–92. <https://doi.org/10.1007/s10694-007-0006-8>
43. Yadav, V. K., Nigam, K., & Srivastava, A. (2020). Forensic investigation of arson residue by infrared and Raman spectroscopy: From conventional to non-destructive techniques. *Medicine, Science and the Law/Medicine, Science and the Law*, 60(3), 206–215. <https://doi.org/10.1177/0025802420914807>
44. Yu, J., Ju, Y., & Gou, X. (2016). Surrogate fuel formulation for oxygenated and hydrocarbon fuels by using the molecular structures and functional groups. *Fuel*, 166, 211–218. <https://doi.org/10.1016/j.fuel.2015.10.08>