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How to Read and Interpret FTIR Spectra for Materials: A Master Dataset with Step-by-Step Guided Peak-Correlation Analysis, Representative Examples, and a Foundation for Future Artificial Intelligence (AI)-Assisted Analysis

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ABSTRACT

Fourier Transform Infrared (FTIR) spectroscopy is widely used for materials characterization; however, spectrum interpretation often relies on isolated peak identification, which can lead to ambiguity, especially for complex materials. This study presents a master FTIR dataset combined with a step-by-step guided peak-correlation workflow to support systematic and reproducible FTIR interpretation. The dataset organizes FTIR information into five spectral regions and emphasizes correlated peak families rather than individual bands. Representative examples covering simple compounds, organic compounds, polymers, and halogenated materials demonstrate the applicability of the approach across materials science and chemical engineering fields. Beyond manual interpretation, the structured dataset and workflow are designed to be machine-readable and extensible, enabling future integration with data-driven methods such as artificial intelligence (AI) and machine learning (ML) for automated spectral analysis. This work provides a practical reference for FTIR interpretation, education, and the development of intelligent materials characterization systems.

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1. INTRODUCTION

Fourier Transform Infrared (FTIR) spectroscopy is widely used for materials characterization due to its rapid and non-destructive identification of molecular structure and chemical bonding (Al-Amin *et al*., 2025; Zhang *et al*., 2021; Barnes *et al*., 2023). However, FTIR spectra are commonly interpreted through isolated peak assignment, which often leads to ambiguity when applied to complex organic, inorganic, or hybrid materials. In practice, FTIR absorptions frequently occur as correlated peak families across multiple spectral regions rather than as independent features. Many reports regarding the FTIR concept and analysis have been well-documented (Berthoumieu & Hienerwadel, 2009; Bacsik *et al*., 2004; Schmitt & Flemming, 1998).

To address this limitation, based on our previous studies on FTIR analysis (Nandiyanto *et al*., 2019; Nandiyanto *et al*., 2023; Nandiyanto *et al*., 2024a; Nandiyanto *et al*., 2024b), this study introduces a master FTIR dataset combined with a step-by-step guided peak-correlation framework that enables systematic interpretation across the full FTIR range (400–4000 cm^{-1}). The novelty of this work lies in organizing FTIR information into correlated peak families with explicit interpretative roles, transforming expert-based interpretation into a reproducible workflow. In addition to supporting manual analysis and education, the structured dataset is designed for future applications, especially providing a foundation for future data-driven and artificial intelligence (AI)-assisted FTIR interpretation in materials science and engineering.

2. CONCEPTUAL FRAMEWORK OF PEAK-CORRELATION IN FTIR

FTIR absorption bands arise from molecular vibrations that are directly related to molecular structure and bonding. Consequently, functional groups typically produce correlated absorptions across multiple spectral regions, forming peak families rather than isolated bands. Interpreting FTIR spectra based solely on individual peak assignment may therefore lead to ambiguity, particularly for complex materials with overlapping or heterogeneous components.

To overcome this limitation, this study adopts a peak-correlation framework in which FTIR spectra are interpreted by identifying related absorptions across the spectrum. The FTIR range is conceptually divided into five interconnected regions, each with a distinct interpretative role, as summarized in **Table 1** and illustrated in **Figure 1**. Within this framework, no single region is interpreted independently; reliable interpretation emerges from consistent peak families observed across regions. This concept provides the basis for the master dataset and the step-by-step interpretation workflow presented in this study.

Table 1. Conceptual division of FTIR spectral regions used in the master dataset.

PART	Wavenumber range (cm^{-1})	Region name	Primary interpretative function	Typical information extracted
PART I	400–700	Low-frequency / heavy-atom region	Final confirmation of heavy atoms and low-frequency modes	Halogen (C–Cl, C–Br, C–I), sulfur species (S–S, C–S), low-frequency out-of-plane vibrations
PART II	700–1500	Fingerprint region	Structural validation and backbone confirmation	C–O, C–N, P–O, S–O, Si–O stretching; skeletal vibrations; aromatic and aliphatic backbone patterns
PART III	1500–1800	Double-bond region	Identification of major functional groups	C=C, C=O, amide bands, aromatic skeletal vibrations
PART IV	1800–2500	Triple-bond and cumulative multiple-bond region	Detection of highly diagnostic, sharp absorptions	C≡C, C≡N, N=C=O, NCS, CO_2, metal carbonyls
PART V	2500–4000	High-frequency single-bond and hydrogen-related region	Rapid assessment of material type and hydrogen bonding	C–H, O–H, N–H stretching; hydrogen bonding effects

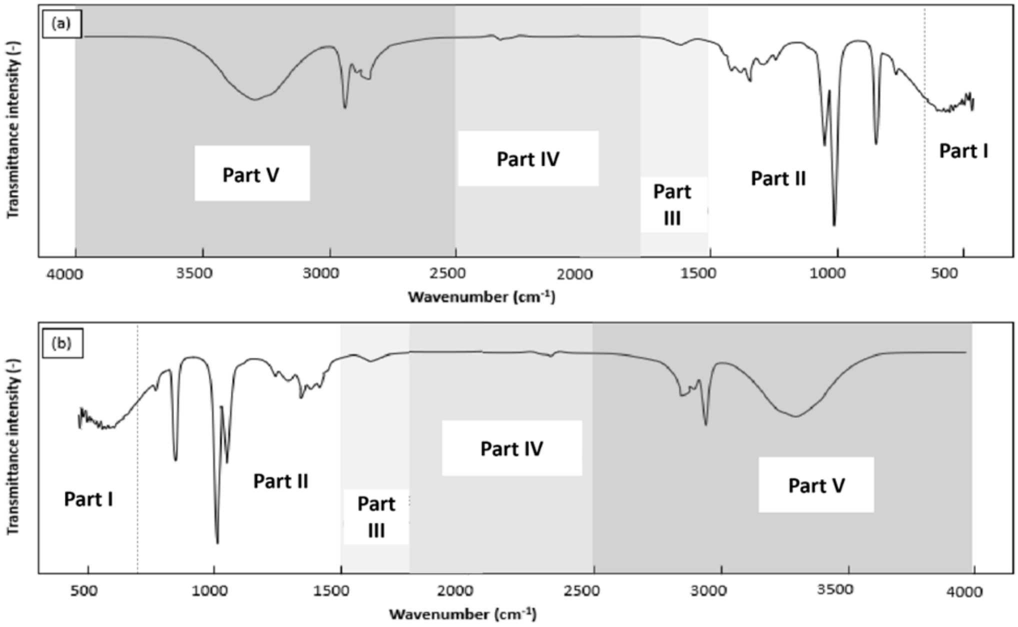

Figure 1. Conceptual illustration of the FTIR spectrum divided into five interconnected regions (PART I–V), highlighting the peak-correlation framework and the integration of peak families across spectral regions for systematic FTIR interpretation: (a) the sequence from 4,000 to 400 cm-1 and (b) the sequence from 400 to 4,000 cm-1. The figure was adopted from reference (Nandiyanto *et al.*, 2023). This figure was selected to verify that the interpretation results obtained using the proposed step-by-step peak-correlation framework are consistent with those reported in the reference.

3. MASTER FTIR DATASET

The master FTIR dataset organizes characteristic absorption bands into five interconnected spectral regions (PART I–V), each with a distinct interpretative role, enabling spectrum interpretation based on correlated peak families rather than isolated bands. Each entry includes the wavenumber range, functional group assignment, peak characteristics, companion peaks, and material classification. The dataset was adopted from the literature (Nandiyanto *et al*., 2019).

In general, PART I (400–700 cm^{-1}) covers low-frequency vibrations involving heavy atoms and out-of-plane modes, providing final confirmation for halogens, sulfur-containing groups, and related signatures (**Table 2**). PART II (700–1500 cm^{-1}) represents the fingerprint region, capturing backbone and heteroatom vibrations (e.g., C–O, C–N, P–O, S–O, Si–O) that validate structural assignments through pattern consistency (**Table 3**). The multiple-bond region is divided into PART III (1500–1800 cm^{-1}), which includes C=C, C=O, amide, and aromatic skeletal vibrations critical for functional group identification (**Table 4**), and PART IV (1800–2500 cm^{-1}), which contains sharp and highly diagnostic triple-bond and cumulative multiple-bond absorptions (**Table 5**). PART V (2500–4000 cm^{-1}) captures single-bond and hydrogen-related stretching modes, providing rapid insight into material type and hydrogen bonding (**Table 6**).

Together, these five regions form an integrated dataset that supports step-by-step FTIR interpretation through peak correlation, forming the basis of the guided workflow described in the following sections.

Table 2. Master FTIR Dataset – PART I (400–700 cm^{-1}): Low-frequency and heavy-atom region. The dataset was adopted and restructured from the literature (Nandiyanto *et al*., 2019).

Wavenumber (cm^{-1})	Functional group/assignment	Peak characteristic	Companion peak(s) / correlated region(s)	Classification
430–500	Aryl disulfide (S–S stretching)	Narrow to medium, often overlapping	600–700 (C–S stretching)	Thiols & sulfur-containing compounds
470–500	Polysulfide (S–S stretching)	Narrow, multiple weak peaks	500–700 (S–S / C–S cluster)	Thiols & sulfur-containing compounds
500–600	Aliphatic iodo compounds (C–I stretching)	Narrow	2850–2950 (aliphatic C–H stretching)	Aliphatic organohalogen compounds
570–705	Disulfide (C–S stretching)	Medium, overlapping	430–500 (S–S stretching)	Thiols & sulfur-containing compounds
590–720	Alcohol O–H out-of-plane bending	Broad	3200–3600 (O–H stretching)	Alcohol & hydroxy compounds
600–620	Disulfide (S–S stretching)	Narrow	570–705 (C–S stretching)	Thiols & sulfur-containing compounds
600–700	Aliphatic bromo compounds (C–Br stretching)	Narrow	2850–2950 (aliphatic C–H stretching)	Aliphatic organohalogen compounds
610–680	Alkyne C–H bending	Narrow	2100–2140 (C≡C stretching); 3310–3320 (≡C–H stretching)	Acetylenic (alkyne) compounds
630	Alkyne C–H bending (typical band)	Sharp, narrow	2100–2140 (C≡C stretching)	Acetylenic (alkyne) compounds
630–660	Thioether (CH_3–S–, C–S stretching)	Narrow to medium	430–500 (S–S stretching); 2850–2950 (C–H stretching)	Thiols & sulfur-containing compounds
670–715	Aryl thioether (Ø–S, C–S stretching)	Medium, overlapping	1500–1600 (aromatic C=C stretching)	Thiols & sulfur-containing compounds
670–900	Aromatic C–H out-of-plane bending	Multiple sharp peaks	1500–1600 (aromatic C=C); 3000–3100 (aromatic C–H stretch)	Aromatic ring compounds
680–610	Sulfate ion (secondary band)	Broad to medium	1080–1130 (sulfate main stretching band)	Inorganic ions
685–710	Thiol / thioether (CH_2–S–, C–S stretching)	Medium	430–500 (S–S stretching); 600–700 (C–S region)	Thiols & sulfur-containing compounds
690–710	Aromatic C–H monosubstitution (phenyl)	Sharp, diagnostic	700–900 (substitution pattern); 1500–1600 (aromatic C=C)	Aromatic ring compounds
700	cis-C–H out-of-plane bending	Narrow	1620–1680 (C=C stretching); 3010–3040 (=C–H stretching)	Olefinic (alkene) compounds

Table 2 (continue). Master FTIR Dataset – PART I (400–700 cm^{-1}): Low-frequency and heavy-atom region. The dataset was adopted and restructured from the literature (Nandiyanto *et al.*, 2019).

Wavenumber (cm^{-1})	Functional group/assignment	Peak characteristic	Companion peak(s) / correlated region(s)	Classification
700–800	Aliphatic chloro compounds (C–Cl stretching)	Narrow	2850–2950 (aliphatic C–H stretching)	Aliphatic organohalogen compounds
700–1300	Skeletal C–C vibrations	Broad, overlapping	2850–2950 (aliphatic C–H stretching)	Saturated aliphatic compounds
720–750	Methylene –$(CH_2)_n$– rocking (n ≥ 3)	Narrow	2850–2950 (long-chain C–H stretching); 1445–1485 (CH_2 bending)	Saturated aliphatic compounds

Table 3. Master FTIR Dataset – PART II (700–1500 cm^{-1}): Fingerprint and heteroatom backbone region. The dataset was adopted and restructured from the literature (Nandiyanto *et al.*, 2019).

Wavenumber (cm^{-1})	Functional group/assignment	Peak characteristic	Companion peak(s) / correlated region(s)	Classification
700–900	Aromatic C–H out-of-plane bending (substitution patterns)	Sharp, multiple	1500–1600 (aromatic C=C); 3000–3100 (aromatic C–H stretch)	Aromatic ring compounds
720–750	Methylene –$(CH_2)_n$– rocking (n ≥ 3)	Narrow, diagnostic	2850–2950 (aliphatic C–H stretch); 1445–1485 (CH_2 bending)	Saturated aliphatic compounds
735–770	Aromatic C–H ortho-disubstitution	Sharp	700–900 (out-of-plane (oop) pattern); 1500–1600 (aromatic C=C)	Aromatic ring compounds
750–810	Aromatic C–H meta-disubstitution	Sharp	700–900 (out-of-plane (oop) pattern); 1500–1600 (aromatic C=C)	Aromatic ring compounds
800–860	Aromatic C–H para-disubstitution	Sharp	700–900 (out-of-plane (oop) pattern); 1500–1600 (aromatic C=C)	Aromatic ring compounds
820–890	Peroxide C–O–O stretching	Weak to medium	1050–1150 (C–O stretch); Raman-active confirmation	Ether & oxy compounds
840–815	Nitrate ion (secondary band)	Medium	1350–1380 (nitrate main band)	Inorganic ions
860–900	Aromatic C–H meta-disubstitution (secondary)	Sharp	1500–1600 (aromatic C=C)	Aromatic ring compounds
880–860	Carbonate ion (secondary band)	Medium	1410–1490 (carbonate main band)	Inorganic ions
900–1000	Silicate ion stretching	Broad	1000–1100 (Si–O main band)	Inorganic ions

Table 3 (continue). Master FTIR Dataset – PART II (700–1500 cm^{-1}): Fingerprint and heteroatom backbone region. The dataset was adopted and restructured from the literature (Nandiyanto *et al.*, 2019).

Wavenumber (cm^{-1})	Functional group/assignment	Peak characteristic	Companion peak(s) / correlated region(s)	Classification
925–1005	Cyclohexane ring vibrations	Medium	2850–2950 (aliphatic C–H); 700–1300 (C–C backbone)	Saturated aliphatic compounds
950–1225	Aromatic C–H in-plane bending	Multiple, overlapping	700–900 (out-of-plane (oop) aromatic); 1500–1600 (aromatic C=C)	Aromatic ring compounds
990–1050	Aliphatic phosphate (P–O–C stretching)	Medium	1250–1350 (P=O stretch)	Phosphorus-oxy compounds
1000–1055	Cyclohexane skeletal vibrations	Medium	700–1300 (C–C backbone); 2850–2950 (C–H stretch)	Saturated aliphatic compounds
1000–1100	Silicate/phosphate ion stretching	Broad	900–1000 (secondary silicate); 1250–1350 (P=O)	Inorganic ions
1000–1150	Aliphatic fluoro compounds (C–F stretching)	Medium to strong	2850–2950 (aliphatic C–H)	Aliphatic organohalogen compounds
1020–1090	Primary amine C–N stretching	Medium	3300–3500 (N–H stretch); 1590–1650 (N–H bending)	Amine compounds
1050	Primary alcohol C–O stretching	Medium	3200–3600 (O–H stretch)	Alcohol & hydroxy compounds
1050–1150	Alkyl ether C–O stretching	Medium	2810–2820 (–O–CH_3 C–H); 2850–2950 (C–H)	Ether & oxy compounds
1070–1140	Cyclic ether (large ring) C–O stretching	Medium	~1250 (epoxy/oxirane companion)	Ether & oxy compounds
1080–1130	Sulfate ion (main band)	Broad, intense	680–610 (secondary sulfate band)	Inorganic ions
1080–1110	Organic siloxane (Si–O–C stretching)	Medium	1020–1055 (Si–O–Si); 1000–1100 (Si–O)	Silicon-oxy compounds
1100	Secondary alcohol C–O stretching	Medium	3200–3600 (O–H stretch)	Alcohol & hydroxy compounds
1130–1190	Secondary amine C–N stretching	Medium	3310–3360 (>N–H stretch)	Amine compounds
1150	Tertiary alcohol C–O stretching	Medium	Weak/absent O–H stretch (free alcohol)	Alcohol & hydroxy compounds
1150–1210	Tertiary amine C–N stretching	Medium	Absence of N–H stretch	Amine compounds
1190–1240	Aromatic phosphate (P–O–C stretching)	Medium	1250–1350 (P=O stretch)	Phosphorus-oxy compounds

Table 3 (continue). Master FTIR Dataset – PART II (700–1500 cm^{-1}): Fingerprint and heteroatom backbone region. The dataset was adopted and restructured from the literature (Nandiyanto *et al*., 2019).

Wavenumber (cm^{-1})	Functional group/assignment	Peak characteristic	Companion peak(s) / correlated region(s)	Classification
1200	Phenol C–O stretching	Medium	3530–3640 (phenolic O–H stretch)	Alcohol & hydroxy compounds
1225–1300	Skeletal C–C vibrations	Broad, overlapping	2850–2950 (aliphatic C–H stretch)	Saturated aliphatic compounds
1230–1270	Aromatic ether (Ar–O stretching)	Medium	1500–1600 (aromatic C=C); 3000–3100 (aromatic C–H)	Ether & oxy compounds
1250	Epoxy/oxirane ring vibration	Medium	820–890 (epoxy companion band)	Ether & oxy compounds
1250–1350	Phosphate P=O stretching	Strong	990–1240 (P–O–C stretching)	Phosphorus-oxy compounds
1260–1350	O–H in-plane bending (primary/secondary alcohol)	Medium	3200–3600 (O–H stretch)	Alcohol & hydroxy compounds
1270–1285	Organic nitrate (secondary band)	Medium	1620–1640 (nitrate asymmetric band)	Nitrogen-oxy compounds
1280–1350	Aromatic secondary amine C–N stretching	Medium	1500–1600 (aromatic C=C); 3300–3500 (N–H)	Amine compounds
1300–1335	Dialkyl/aryl sulfone stretching	Medium	1170–1135 (SO_2 symmetric band)	Sulfur-oxy compounds
1310–1410	Phenol / tertiary alcohol O–H bending	Broad	3200–3600 (O–H stretch)	Alcohol & hydroxy compounds
1320–1355	Nitro compound symmetric stretching	Strong	1485–1555 (NO_2 asymmetric stretch)	Nitrogen-oxy compounds
1340–1365	Sulfonate stretching	Medium	1100–1200 (S–O region)	Sulfur-oxy compounds
1350–1380	Nitrate ion (main band)	Strong	840–815 (secondary nitrate band)	Inorganic ions
1370–1420	Organic sulfate stretching	Medium	1080–1130 (sulfate main band)	Sulfur-oxy compounds
1380–1385	Methyl symmetric bending (–CH_3)	Medium	2850–2950 (C–H stretch)	Saturated aliphatic compounds
1410–1490	Carbonate ion (main band)	Strong	880–860 (secondary carbonate band)	Inorganic ions
1410–1420	Vinyl C–H in-plane bending	Medium	1620–1680 (C=C stretch)	Olefinic (alkene) compounds
1430–1470	Methyl asymmetric bending (–CH_3)	Medium	2850–2970 (C–H stretch)	Saturated aliphatic compounds

Table 3 (continue). Master FTIR Dataset – PART II (700–1500 cm^{-1}): Fingerprint and heteroatom backbone region. The dataset was adopted and restructured from the literature (Nandiyanto *et al*., 2019).

Wavenumber (cm^{-1})	Functional group/assignment	Peak characteristic	Companion peak(s) / correlated region(s)	Classification
1445–1485	Methylene C–H bending (>CH_2)	Medium	2850–2950 (C–H stretch)	Saturated aliphatic compounds
1450–1510	Aromatic ring skeletal stretching	Medium	1580–1615 (aromatic C=C)	Aromatic ring compounds
1485–1555	Nitro compound asymmetric stretching	Strong	1320–1355 (NO_2 symmetric stretch)	Nitrogen-oxy compounds

Table 4. Master FTIR Dataset – PART III (1500–1800 cm^{-1}): Double-bond region. The dataset was adopted and restructured from the literature (Nandiyanto *et al*., 2019).

Wavenumber (cm^{-1})	Functional group/assignment	Peak characteristic	Companion peak(s) / correlated region(s)	Classification
1500–1510	Aromatic ring skeletal stretching	Medium	1580–1615 (aromatic C=C); 700–900 (aromatic C–H out-of-plane)	Aromatic ring compounds
1500–1650	Aromatic C=C stretching	Medium to sharp	3000–3100 (aromatic C–H stretching); 700–900 (out-of-plane (oop) bending)	Aromatic ring compounds
1510–1550	Nitro compound asymmetric stretching (–NO_2)	Strong, sharp	1320–1355 (NO_2 symmetric stretching)	Nitrogen-oxy compounds
1550–1610	Carboxylate ion (COO^-) asymmetric stretching	Strong	1300–1420 (COO^- symmetric stretching)	Carboxylate / carbonyl-related compounds
1575–1630	Azo group (–N=N– stretching)	Medium	Conjugated aromatic C=C bands (1500–1600)	Nitrogen multiple-bond compounds
1580–1615	Aromatic ring C=C–C skeletal vibration	Sharp	700–900 (aromatic out-of-plane (oop)); 3000–3100 (aromatic C–H)	Aromatic ring compounds
1590–1690	Imino group (C=N stretching)	Medium	3300–3500 (=N–H stretching, if present)	Nitrogen multiple-bond compounds
1600–1650	Conjugated C=C stretching (alkene/aromatic conjugation)	Medium	3010–3040 (=C–H stretching)	Olefinic (alkene) compounds
1620–1640	Organic nitrate asymmetric stretching	Medium	1270–1285 (nitrate secondary band)	Nitrogen-oxy compounds
1620–1670	Unsaturated C=C (general)	Medium	3010–3095 (=C–H stretching); 700–1000 (bending modes)	Unsaturated compounds

Table 4 (continue). Master FTIR Dataset – PART III (1500–1800 cm^{-1}): Double-bond region. The dataset was adopted and restructured from the literature (Nandiyanto *et al*., 2019).

Wavenumber (cm^{-1})	Functional group/assignment	Peak characteristic	Companion peak(s) / correlated region(s)	Classification
1650	Olefinic C=C stretching	Sharp	3010–3040 (=C–H stretching)	Olefinic (alkene) compounds
1650–1680	Amide I (C=O stretching)	Strong	1550–1650 (Amide II: N–H bending)	Amide compounds
1675–1690	Quinone or conjugated ketone C=O stretching	Strong	Lower-frequency shift compared to saturated ketones	Carbonyl compounds
1700–1725	Carboxylic acid C=O stretching	Strong, broad	2500–3300 (very broad O–H stretching)	Carbonyl compounds
1705–1725	Ketone C=O stretching	Strong, sharp	Absence of broad O–H stretching	Carbonyl compounds
1725–1740	Aldehyde C=O stretching	Strong	2700–2800 (aldehyde C–H stretching)	Carbonyl compounds
1725–1750	Ester C=O stretching	Strong	1000–1300 (C–O stretching)	Carbonyl compounds
1735	Six-membered ring lactone C=O	Strong	Characteristic fingerprint bands (1000–1300)	Carbonyl compounds
1740–1760	Alkyl carbonate C=O stretching	Strong	1050–1250 (C–O–C stretching)	Carbonate compounds
1770–1815	Acid (acyl) halide C=O stretching	Strong	600–800 (C–X halogen stretching)	Carbonyl compounds
1775–1820	Aryl carbonate C=O stretching	Strong	1500–1600 (aromatic C=C stretching)	Carbonate compounds
1820–1870	Anhydride C=O (high-frequency band)	Strong (often doublet)	1775–1800 (second anhydride band)	Carbonyl compounds

Table 5. Master FTIR Dataset – PART IV (1800–2500 cm^{-1}): Triple-bond and cumulative multiple-bond region. The dataset was adopted and restructured from the literature (Nandiyanto *et al*., 2019).

Wavenumber (cm^{-1})	Functional group/assignment	Peak characteristic	Companion peak(s) / correlated region(s)	Classification
1800–2100	Transition metal carbonyls (M–CO stretching)	Strong, sharp	Metal–ligand specific bands; environment-dependent shifts	Inorganic/organometallic compounds
1820–1870	Anhydride C=O (low-frequency band)	Strong (doublet component)	1775–1800 (high-frequency anhydride band)	Carbonyl compounds
1870–1800	Anhydride C=O (high-frequency band)	Strong (doublet component)	1820–1870 (low-frequency anhydride band)	Carbonyl compounds
1990–2150	Isothiocyanate (–NCS stretching)	Medium	2100–2260 (C≡C / C≡N comparison region)	Nitrogen–sulfur compounds
2000–2200	Cyanide/thiocyanate ions	Medium to sharp	Comparison with organic nitrile patterns	Inorganic ions
2100–2140	Terminal alkyne C≡C stretching	Medium	3310–3320 (≡C–H stretching)	Acetylenic (alkyne) compounds
2140–2175	Thiocyanate (–SCN stretching)	Medium	2220–2240 (C≡N stretching)	Nitrogen–sulfur compounds
2190–2260	Medial (disubstituted) alkyne C≡C stretching	Medium	Absence of ≡C–H stretching (3310–3320)	Acetylenic (alkyne) compounds
2220–2240	Aromatic nitrile (C≡N stretching)	Sharp, strong	1500–1600 (aromatic C=C stretching)	Nitrogen multiple-bond compounds
2240–2260	Cyanate (–OCN stretching)	Medium	1080–1190 (C–O stretching)	Nitrogen–oxy compounds
2240–2276	Isocyanate (–N=C=O asymmetric stretching)	Strong	~1700 (carbonyl-related band)	Nitrogen multiple-bond compounds
2240–2280	Aliphatic nitrile (C≡N stretching)	Sharp	2850–2950 (aliphatic C–H stretching)	Nitrogen multiple-bond compounds
2330–2360	Carbon dioxide (CO_2 asymmetric stretching)	Sharp, narrow	Environmental/background reference	Inorganic/gaseous species
2350	Graphitic carbon / CO_2-related absorption	Weak to medium	Sample atmosphere, baseline context	Carbon / particle-related compounds
2400–2500	Weak overtone/combination bands	Weak, broad	Context-dependent; rarely diagnostic alone	Combination bands

Table 6. Master FTIR Dataset – PART V (2500–4000 cm^{-1}): High-frequency single-bond and hydrogen-related region. The dataset was adopted and restructured from the literature (Nandiyanto *et al*., 2019).

Wavenumber (cm^{-1})	Functional group/assignment	Peak characteristic	Companion peak(s) / correlated region(s)	Classification
2500–2700	Carboxylic acid O–H stretching	Very broad, intense	1700–1725 (acid C=O stretching); 1200–1320 (C–O stretching, often present)	Carbonyl compounds
2700–2800	Aldehyde C–H stretching	Weak to medium, narrow	1725–1740 (aldehyde C=O stretching)	Carbonyl compounds
2780–2820	Methylamino / N–CH_3 C–H stretching	Narrow	1000–1210 (C–N stretching); 1550–1650 (N–H bending, if N–H exists)	Amine compounds
2810–2820	Methoxy (–O–CH_3) C–H stretching	Narrow	1050–1150 (C–O stretching); 2820–2810 (paired methoxy band, if resolved)	Ether & oxy compounds
2815–2850	Methoxy/methyl ether C–H stretching	Narrow	1050–1150 (C–O stretching)	Ether & oxy compounds
2845–2865	Methylene C–H symmetric stretching	Sharp	2915–2935 (CH_2 asymmetric stretch); 1445–1485 (CH_2 bending)	Saturated aliphatic compounds
2860–2880	Methyl C–H symmetric stretching	Sharp	2950–2970 (CH_3 asymmetric stretch); 1370–1385 (CH_3 bending)	Saturated aliphatic compounds
2880–2900	Methyne (>CH–) C–H stretching	Sharp	1350–1330 (methyne C–H bending); 700–1300 (skeletal C–C)	Saturated aliphatic compounds
2915–2935	Methylene C–H asymmetric stretching	Strong, sharp	2845–2865 (CH_2 symmetric stretch); 1445–1485 (CH_2 bending)	Saturated aliphatic compounds
2950–2970	Methyl C–H asymmetric stretching	Strong, sharp	2860–2880 (CH_3 symmetric stretch); 1430–1470 & 1370–1385 (CH_3 bending)	Saturated aliphatic compounds
3000–3150	Aromatic C–H stretching	Sharp	1500–1600 (aromatic C=C stretching); 700–900 (aromatic C–H out-of-plane (oop))	Aromatic ring compounds
3010–3040	Olefinic (=C–H) stretching	Sharp	1620–1680 (C=C stretching); 700–1000 (=C–H bending region)	Olefinic (alkene) compounds
3075–3095	Vinyl/vinylidene C–H stretching	Sharp	900–1000 (vinyl/vinylidene bending patterns); 1620–1680 (C=C)	Olefinic (alkene) compounds
3200–3400	Hydrogen-bonded O–H stretching	Broad	1260–1410 (O–H bending); 1050–1200 (C–O stretching, if alcohol/phenol)	Alcohol & hydroxy compounds
3200–3570	Hydroxy group (H-bonded O–H)	Very broad	1260–1410 (O–H bending)	Alcohol & hydroxy compounds

Table 6 (continue). Master FTIR Dataset – PART V (2500–4000 cm^{-1}): High-frequency single-bond and hydrogen-related region. The dataset was adopted and restructured from the literature (Nandiyanto *et al*., 2019).

Wavenumber (cm^{-1})	Functional group/assignment	Peak characteristic	Companion peak(s) / correlated region(s)	Classification
3310–3320	Terminal alkyne ≡C–H stretching	Sharp	2100–2140 (terminal C≡C stretching)	Acetylenic (alkyne) compounds
3310–3360	Secondary amine >N–H stretching	Medium	1550–1650 (N–H bending); 1130–1190 (C–N stretching)	Amine compounds
3320–3350	Imino (=N–H) stretching	Medium	1590–1690 (C=N stretching)	Nitrogen multiple-bond compounds
3380–3400	Primary amine N–H stretching (aliphatic)	Medium (often doublet)	1590–1650 (NH_2 bending); 1020–1090 (C–N stretching)	Amine compounds
3380–3415	Primary amine N–H stretching (aromatic)	Medium (often doublet)	1500–1600 (aromatic C=C); 1590–1650 (NH_2 bending)	Amine compounds
3430–3490	Heterocyclic amine >N–H stretching	Medium	1550–1650 (N–H bending)	Amine compounds
3450–3550	Dimeric O–H stretching	Broad	1260–1410 (O–H bending); 1050–1200 (C–O stretching)	Alcohol & hydroxy compounds
3530–3640	Phenolic O–H stretching	Medium to sharp	1200 (phenol C–O stretching); 1500–1600 (aromatic C=C)	Alcohol & hydroxy compounds
3540–3570	Internally bonded O–H stretching	Narrow	Weaker broad O–H region compared to H-bonded	Alcohol & hydroxy compounds
3600–3645	Nonbonded / “free” O–H stretching	Sharp, narrow	Often reduced O–H bending signature	Alcohol & hydroxy compounds
3620–3635	Secondary alcohol O–H stretching	Sharp	1100 (secondary alcohol C–O stretching)	Alcohol & hydroxy compounds
3630–3645	Primary alcohol O–H stretching	Sharp	1050 (primary alcohol C–O stretching)	Alcohol & hydroxy compounds

4. STEP-BY-STEP INTERPRETATION WORKFLOW USING THE MASTER FTIR DATASET

The master FTIR dataset is intended to be applied through a clear, sequential workflow that emphasizes correlated peak families across the five spectral regions (PART I–V). The following numbered steps provide a practical procedure that can be directly implemented for routine materials analysis. The numbered workflow is summarized in **Table 7**. By following these steps sequentially, FTIR spectra can be interpreted transparently and reproducibly, minimizing ambiguity and reducing the risk of misassignment through isolated peak reading.

(i) **Step 0. Pre-check of spectral quality**. Begin by confirming that the FTIR spectrum is suitable for interpretation. Verify the wavenumber orientation (typically 4000–400 cm^{-1}), identify the acquisition mode (ATR or transmission), and inspect baseline stability and noise levels. Apply baseline correction if required. This step prevents artefacts from influencing subsequent assignments.

(ii) **Step 1. High-frequency region—initial material screening (PART V, 2500–4000 cm^{-1})**. Examine C–H, O–H, and N–H stretching bands to obtain rapid insight into the general chemical nature of the material. Sharp bands at 2850–2970 cm^{-1} indicate aliphatic C–H, while bands above 3000 cm^{-1} suggest aromatic or olefinic C–H. Broad absorptions between 3200 and 3600 cm^{-1} are characteristic of O–H stretching and hydrogen bonding, whereas medium-intensity bands or doublets in this region often indicate N–H stretching. At this stage, note expected companion peaks in lower regions (e.g., carbonyl or fingerprint features) without drawing final conclusions.

(iii) **Step 2. Double-bond region—identification of major functional groups (PART III, 1500–1800 cm^{-1})**. Inspect absorptions associated with C=C and C=O functionalities. Aromatic skeletal vibrations and conjugated C=C bands typically appear between 1500 and 1650 cm^{-1}, while carbonyl groups produce strong bands in the 1650–1800 cm^{-1} range. Use band position and shape to distinguish among ketones, aldehydes, esters, carboxylic acids, amides, and related groups. Confirm assignments by checking correlated features, such as O–H stretching for carboxylic acids or C–O stretching for esters.

(iv) **Step 3. Triple-bond and cumulative multiple-bond region—diagnostic confirmation (PART IV, 1800–2500 cm^{-1}).** Evaluate this region for sharp and well-isolated absorptions, including nitriles (C≡N), alkynes (C≡C), isocyanates (N=C=O), and related species. When present, these bands provide strong confirmatory evidence. Correlate terminal alkyne bands with ≡C–H stretching near 3300 cm^{-1} and aromatic nitriles with aromatic skeletal features. The absence of peaks here does not negate other assignments but helps constrain structural possibilities.

(v) **Step 4. Fingerprint region—structural validation (PART II, 700–1500 cm^{-1})**. Use the fingerprint region to validate and refine assignments made in Steps 1–3. Identify consistent patterns of C–O, C–N, P–O, S–O, and Si–O stretching, along with backbone skeletal vibrations. Individual bands are rarely diagnostic; interpretation relies on pattern consistency. For example, ester carbonyls should be supported by characteristic C–O bands, while sulfate or carbonate assignments require the expected combination of main and secondary absorptions.

(vi) **Step 5. Low-frequency region—final supporting evidence (PART I, 400–700 cm^{-1})**. Finally, examine low-frequency absorptions to confirm heavy-atom signatures and out-of-plane modes, such as halogenated groups or sulfur-containing species. Although rarely used as primary identifiers, these bands provide valuable supporting evidence that strengthens the overall interpretation when consistent with higher-frequency assignments.

Table 7. Numbered step-by-step FTIR interpretation workflow based on the master dataset

Step	FTIR region (PART)	Primary purpose	Typical outputs
0	Pre-check	Ensure spectral quality and correct orientation	Baseline-corrected, reliable spectrum
1	PART V (2500–4000)	Rapid screening of C–H, O–H, N–H	Initial material classification
2	PART III (1500–1800)	Identify C=C and C=O functionalities	Major functional groups
3	PART IV (1800–2500)	Detect triple-bond and cumulative species	Highly diagnostic confirmation
4	PART II (700–1500)	Validate structure via fingerprint patterns	Consistency and refinement
5	PART I (400–700)	Confirm heavy atoms and low-frequency modes	Final supporting evidence

5. REPRESENTATIVE EXAMPLE: STEP-BY-STEP FTIR INTERPRETATION

To simplify the illustration of the proposed step-by-step FTIR interpretation workflow, representative spectra in this section are adopted from an open-access FTIR reference database for conservation and materials analysis (https://spectra.chem.ut.ee/conservation_materials/ and https://orgchemboulder.com/Spectroscopy/irtutor/alkhalidesir.shtml; accessed and updated on 11 January 2026). The use of standardized reference spectra allows a clear demonstration of the master dataset and peak-correlation approach.

5.1. Case 1: Inorganic / silicate-type with hydroxyl material

The FTIR spectrum of the representative material is shown in **Figure 2** and is interpreted using the step-by-step workflow based on the master FTIR dataset.

(i) **Step 0. Spectral quality check.** The spectrum covers the full FTIR range (4000–400 cm^{-1}) with a stable baseline and low noise. No significant artefacts are observed, indicating that the spectrum is suitable for interpretation. The extracted absorption peaks used as the basis for the step-by-step analysis are summarized in **Table 8**.

(ii) **Step 1. High-frequency region (PART V, 2500–4000 cm^{-1}).** A broad and strong absorption band is observed at approximately 3260 cm^{-1}, which is characteristic of O–H stretching associated with hydrogen-bonded hydroxyl groups or adsorbed water. No distinct absorption bands are detected in the aliphatic C–H stretching region (2850–2970 cm^{-1}), indicating that organic hydrocarbon components are not dominant in the material.

(iii) **Step 2. Double-bond region (PART III, 1500–1800 cm^{-1}).** An absorption band appears at approximately 1635 cm^{-1}. When correlated with the broad O–H stretching band at higher wavenumber, this feature is consistent with H–O–H bending vibrations, which are commonly associated with molecular or bound water in inorganic or particulate materials. No strong carbonyl-related absorptions are detected in this region.

(iv) **Step 3. Triple-bond and cumulative multiple-bond region (PART IV, 1800–2500 cm^{-1}).** No significant absorption bands are present in this region, excluding the presence of triple-bond or cumulative multiple-bond functionalities such as nitriles, alkynes, or isocyanates.

(v) **Step 4. Fingerprint region (PART II, 700–1500 cm^{-1}).** A broad and intense absorption band is observed in the range of approximately 1000–1100 cm^{-1}, which is characteristic of Si–O stretching vibrations in silicate or metal–oxygen frameworks. This band represents the dominant backbone vibration of the material and serves as a key fingerprint feature for inorganic network structures.

(vi) **Step 5. Low-frequency region (PART I, 400–700 cm^{-1}).** Weaker but distinct absorption bands are observed at approximately 490 and 401 cm^{-1}. These low-frequency features are consistent with Si–O bending modes and/or metal–oxygen lattice vibrations, providing additional supporting evidence for an inorganic framework.

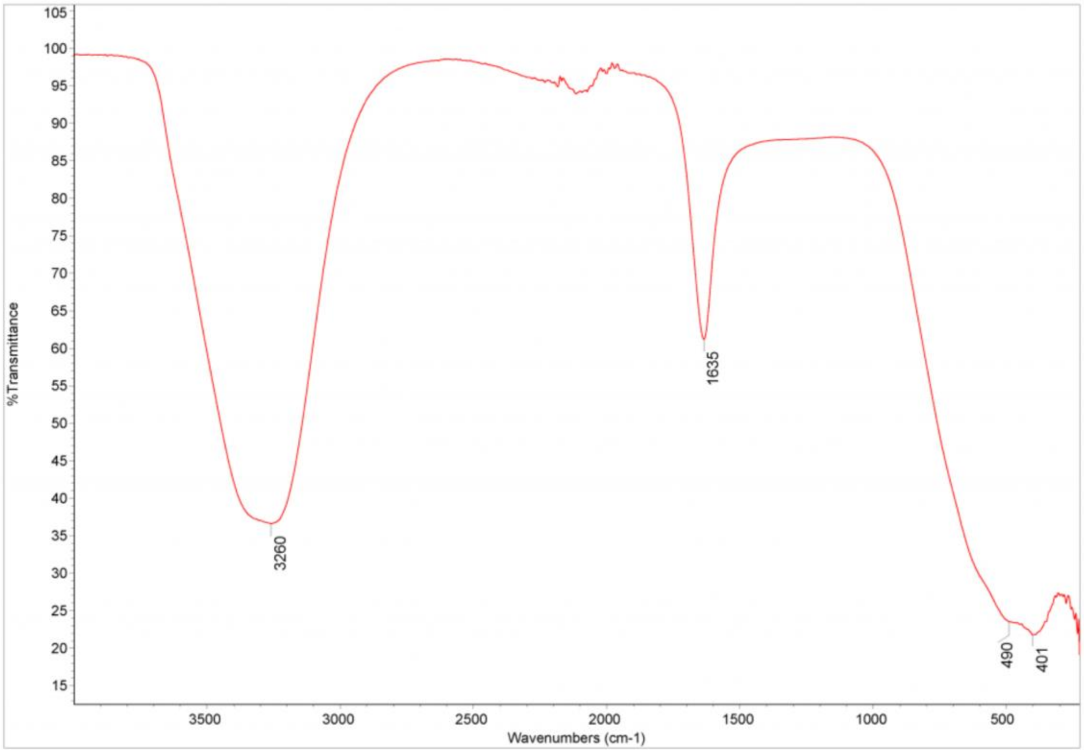

Figure 2. FTIR spectrum of a representative material, Case 1. The figure was adopted from reference (https://spectra.chem.ut.ee/conservation_materials/; accessed and updated on 11 January 2026).

Table 8. Extracted FTIR peaks from Figure 2 used for step-by-step interpretation

No	Experimental data			Wavenumber in reference (cm⁻¹)	Companion peak(s)	Assignment	Interpretation role
	Approx. wavenumber (cm^{-1})	Peak characteristic	Part				
1	~3260	Broad, strong	V	3200–3600	Peak No. 2 (H–O–H bending at ~1635) for O–H / water confirmation	O–H stretching (hydrogen-bonded)	Identifies hydroxyl groups or adsorbed water
2	~1635	Sharp, medium	III	1600–1650	Peak No. 1 (O–H stretching at ~3260) to confirm bound or adsorbed water	H–O–H bending vibration	Confirms the presence of molecular or bound water
3	~1100–1000	Broad, strong	II	1000–1100	Peaks No. 4 & 5 (low-frequency Si–O bending/lattice modes) for framework validation	Si–O stretching (silicate framework)	Main backbone vibration in the fingerprint region
4	~490	Sharp, weak	I	450–520	Peak No. 3 (Si–O stretching at ~1100–1000) for bending–stretching correlation	Si–O bending vibration	Supporting evidence for silicate-type structure
5	~401	Sharp, weak	I	380–450	Peak No. 3 (Si–O stretching at ~1100–1000) to confirm metal–oxygen lattice	Metal–O or lattice vibration	Final confirmation of the inorganic framework

5.2. Case 2: Simple carbonyl

The FTIR spectrum of the representative organic material is shown in **Figure 3** and is interpreted using the step-by-step workflow based on the master FTIR dataset.

(i) **Step 0. Spectral quality check.** The spectrum covers the full FTIR range (4000–400 cm^{-1}) with a stable baseline and clearly resolved absorption bands. No significant artefacts are observed, indicating that the spectrum is suitable for step-by-step interpretation. The extracted absorption peaks used for analysis are summarized in **Table 9**.

(ii) **Step 1. High-frequency region (PART V, 2500–4000 cm^{-1}).** A weak and broad absorption band is observed at approximately 3412 cm^{-1}, suggesting the presence of O–H stretching, likely associated with weakly hydrogen-bonded hydroxyl groups or residual moisture. In addition, a distinct absorption at approximately 3004 cm^{-1} corresponds to aromatic or olefinic C–H stretching. The coexistence of these bands indicates that the material contains unsaturated organic components with possible hydroxyl involvement.

(iii) **Step 2. Double-bond region (PART III, 1500–1800 cm^{-1}).** A very strong and sharp absorption band is observed in the range of 1710–1749 cm^{-1}, which is characteristic of carbonyl (C=O) stretching. The position and intensity of this band are consistent with an ester-type carbonyl rather than a carboxylic acid or amide, as no broad O–H band typical of acids or amide-related features are present.

(iv) **Step 3. Triple-bond and cumulative multiple-bond region (PART IV, 1800–2500 cm^{-1}).** No significant absorption bands are detected in this region, excluding the presence of triple-bond or cumulative multiple-bond functionalities such as nitriles or alkynes. This simplifies the interpretation by limiting the functional group possibilities.

(v) **Step 4. Fingerprint region (PART II, 700–1500 cm^{-1}).** The fingerprint region displays multiple absorption bands, including peaks at approximately 1436, 1420, and 1358 cm^{-1}, which are associated with bending vibrations of alkyl (–CH_2/–CH_3) groups. Strong bands at approximately 1220, 1092, and 1059 cm^{-1} are assigned to C–O stretching vibrations, providing strong supporting evidence for ester linkages within the organic structure. Additional bands at approximately 902 and 786 cm^{-1} correspond to out-of-plane C–H bending modes, supporting the presence of aromatic or unsaturated groups.

(vi) **Step 5. Low-frequency region (PART I, 400–700 cm^{-1}).** Weak but distinct absorption bands are observed at approximately 529, 492, and 392 cm^{-1}. These low-frequency features are attributed to skeletal or ring deformation modes and provide final supporting evidence for the organic framework.

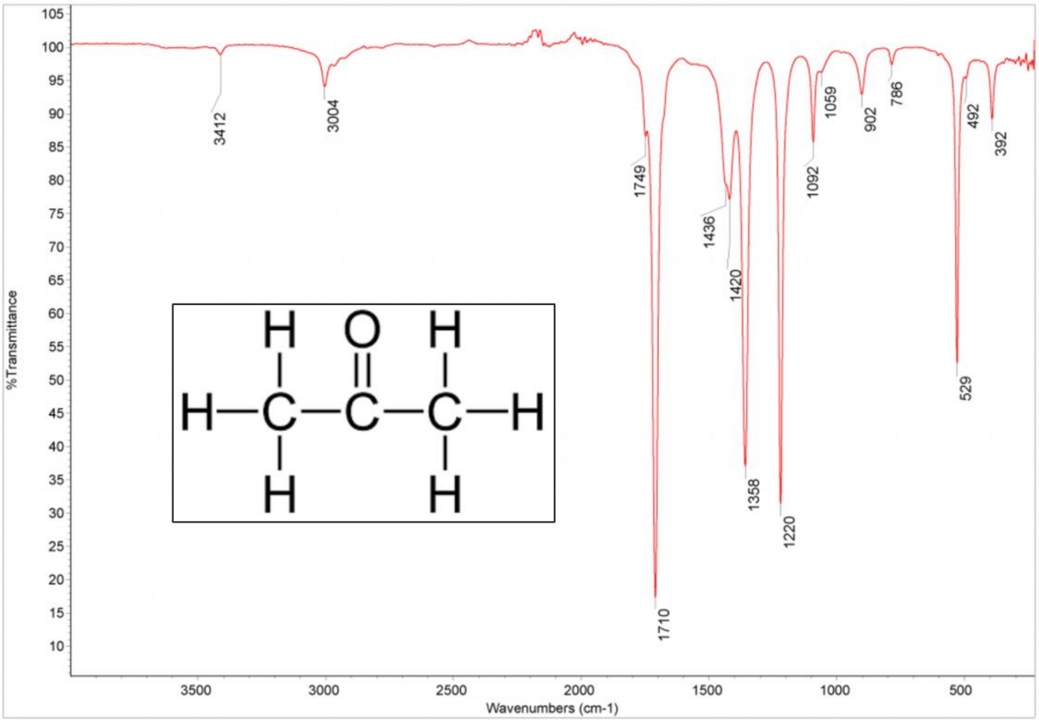

Figure 3. FTIR spectrum of a representative material, Case 2. The figure was adopted from reference (https://spectra.chem.ut.ee/conservation_materials/; accessed and updated on 11 January 2026).

Table 9. Extracted FTIR peaks from Figure 3 used for step-by-step interpretation

No	Experimental data			Wavenumber in reference (cm^{-1})	Companion peak(s)	Assignment	Interpretation role
	Approx. wavenumber (cm^{-1})	Peak characteristic	Part				
1	~3412	Broad, weak–medium	V	3200–3600	Peak No. 2 (~3004) to check aromatic/olefinic vs O–H	O–H stretching (weakly hydrogen-bonded)	Indicates possible hydroxyl or moisture
2	~3004	Sharp, weak	V	3000–3100	Peak No. 6–7 (C=C related) for aromatic confirmation	Aromatic/olefinic C–H stretching	Indicates unsaturated or aromatic C–H
3	~1749–1710	Very strong, sharp	III	1700–1750	Peaks No. 6–8 (C–O stretching region) for ester validation	C=O stretching (ester/carbonyl)	Primary functional group identification
4	~1436	Medium	II	1400–1460	Peak No. 5 (~1420) for CH bending pair	CH_2 / CH_3 bending	Fingerprint support for alkyl groups
5	~1420	Medium	II	1410–1440	Peak No. 4 (~1436) for CH bending correlation	CH_2 / CH_3 bending	Confirms alkyl substituents
6	~1358	Medium	II	1340–1380	Peak No. 4–5 (alkyl bending)	CH_3 symmetric bending	Fingerprint alkyl confirmation
7	~1220	Strong, sharp	II	1200–1300	Peak No. 3 (C=O) for ester linkage check	C–O stretching (ester)	Supports ester functionality
8	~1092	Medium	II	1050–1150	Peak No. 7 (~1220)	C–O stretching	Additional ester fingerprint
9	~1059	Medium	II	1020–1080	Peak No. 7–8 (C–O region)	C–O stretching	Confirms oxygenated backbone
10	~902	Sharp, weak	II	880–910	Peak No. 2 (~3004)	=C–H out-of-plane bending	Aromatic/olefinic confirmation
11	~786	Sharp, weak	II	750–820	Peak No. 2 (~3004)	Aromatic C–H out-of-plane	Aromatic ring support
12	~529	Sharp, weak	I	500–550	Peak No. 3 (C=O) for framework check	Skeletal / ring deformation	Low-frequency organic support
13	~492	Sharp, weak	I	450–520	Peak No. 12 (~529)	Skeletal vibration	Supporting low-frequency mode
14	~392	Sharp, weak	I	380–420	Peak No. 12–13	Lattice / skeletal vibration	Final low-frequency confirmation

5.3. Case 3: Aromatic / substituted organic material

The FTIR spectrum of the representative material is shown in **Figure 4** and is interpreted using the step-by-step workflow based on the master FTIR dataset.

(i) **Step 0. Spectral quality check.** The spectrum covers the full FTIR range (4000–400 cm^{-1}) with a stable baseline and well-resolved absorption bands. Numerous sharp peaks are observed across multiple regions, indicating high spectral quality and suitability for detailed step-by-step interpretation. The extracted absorption peaks used for analysis are summarized in **Table 10**.

(ii) **Step 1. High-frequency region (PART V, 2500–4000 cm^{-1}).** Several absorption bands are observed in the region above 3000 cm^{-1}, including peaks at approximately 3085, 3061, and 3026 cm^{-1}, which are characteristic of aromatic C–H stretching vibrations. Additional bands at approximately 2949, 2919, and 2871 cm^{-1} correspond to aliphatic C–H stretching. A weak feature near 2733 cm^{-1} may be associated with overtone or combination bands. The coexistence of aromatic and aliphatic C–H stretching indicates an aromatic-rich organic structure with alkyl substituents.

(iii) **Step 2. Double-bond region (PART III, 1500–1800 cm^{-1}).** Multiple absorption bands are observed in this region, including peaks at approximately 1623 and 1604 cm^{-1}, which are characteristic of aromatic C=C stretching vibrations. Additional bands at approximately 1572 cm^{-1} further support the presence of an aromatic ring system. No dominant carbonyl absorption is observed near 1700–1750 cm^{-1}, indicating that carbonyl functionalities are not a major component of this material.

(iv) **Step 3. Triple-bond and cumulative multiple-bond region (PART IV, 1800–2500 cm^{-1}).** No strong diagnostic absorption bands are present in the 1800–2500 cm^{-1} range. This excludes the presence of nitrile, alkyne, or other cumulative multiple-bond functionalities and simplifies the structural interpretation.

(v) **Step 4. Fingerprint region (PART II, 700–1500 cm^{-1}).** The fingerprint region exhibits numerous well-defined absorption bands. Peaks at approximately 1495 and 1459 cm^{-1} correspond to aromatic ring skeletal vibrations. Strong bands at approximately 1248, 1209, 1178, 1106, 1081, and 1030 cm^{-1} are associated with in-plane C–H bending and ring-related vibrations. Additional bands at approximately 895, 843, 785, and 692 cm^{-1} are assigned to out-of-plane aromatic C–H bending modes, which are highly diagnostic for substituted aromatic systems.

(vi) **Step 5. Low-frequency region (PART I, 400–700 cm^{-1}).** Distinct absorption bands are observed at approximately 725, 621, 521, 463, and 345 cm^{-1}. These low-frequency features are attributed to ring deformation, skeletal vibrations, and lattice-related modes, providing final supporting evidence for a rigid aromatic framework.

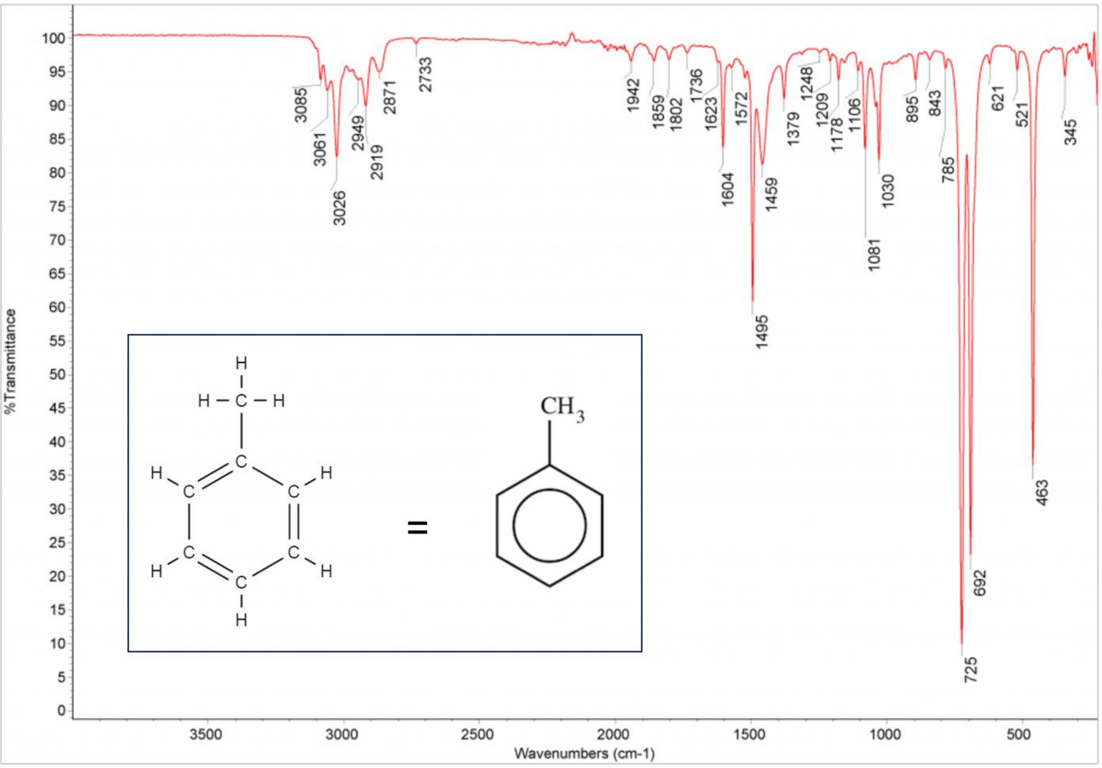

Figure 4. FTIR spectrum of a representative material, Case 3. The figure was adopted from reference (https://spectra.chem.ut.ee/conservation_materials/; accessed and updated on 11 January 2026).

5.4. Case 4: Simple Hydroxyl Material with Alkyl and Ether Features

The FTIR spectrum of the representative material is shown in **Figure 5** and is interpreted using the step-by-step workflow based on the master FTIR dataset.

(o) **Step 0. Spectral quality check.** The spectrum covers the full FTIR range (4000–400 cm^{-1}) with a stable baseline and clearly distinguishable absorption bands. The spectrum quality is sufficient for systematic interpretation. The extracted absorption peaks used as the basis for analysis are summarized in **Table 11**.

(i) **Step 1. High-frequency region (PART V, 2500–4000 cm^{-1}).** A broad and intense absorption band is observed at approximately 3316 cm^{-1}, which is characteristic of O–H stretching associated with hydrogen-bonded hydroxyl groups. In addition, multiple sharp absorption bands are present at approximately 2973, 2927, and 2881 cm^{-1}, corresponding to aliphatic C–H stretching vibrations. The coexistence of strong O–H and aliphatic C–H bands indicates a hydroxylated organic material with an alkyl backbone.

(ii) **Step 2. Double-bond region (PART III, 1500–1800 cm^{-1}).** An absorption band is observed at approximately 1655 cm^{-1}. When correlated with the strong O–H stretching band at higher wavenumber, this feature is consistent with H–O–H bending or hydrogen-bond-related deformation rather than a carbonyl (C=O) stretching vibration. No strong ester or ketone carbonyl absorption is detected near 1700–1750 cm^{-1}.

(iii) **Step 3. Triple-bond and cumulative multiple-bond region (PART IV, 1800–2500 cm^{-1}).** No significant absorption bands are detected in this region, excluding the presence of triple-bond or cumulative multiple-bond functionalities such as nitriles or alkynes.

(iv) **Step 4. Fingerprint region (PART II, 700–1500 cm^{-1}).** The fingerprint region shows several well-defined absorption bands. Peaks at approximately 1454, 1420, 1379, and 1327 cm^{-1} are attributed to bending vibrations of alkyl ($-CH_2/-CH_3$) groups. Strong absorptions at approximately 1273, 1087, and 1045 cm^{-1} are assigned to C–O stretching vibrations, indicating the presence of ether or alcohol functionalities within the organic framework. An additional band near 880 cm^{-1} corresponds to C–H out-of-plane bending.

(v) **Step 5. Low-frequency region (PART I, 400–700 cm^{-1}).** Absorption bands at approximately 626 and 431 cm^{-1} are observed in the low-frequency region and are associated with skeletal or deformation modes, providing supporting evidence for the organic framework.

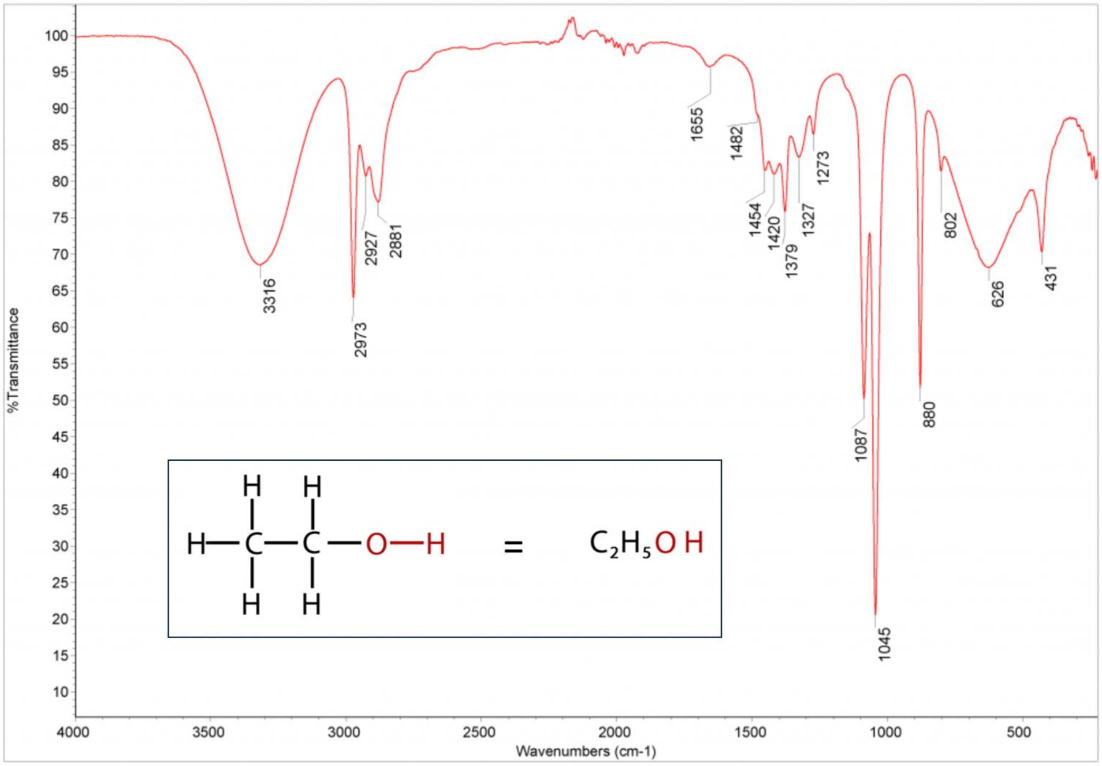

Figure 5. FTIR spectrum of a representative material, Case 4. The figure was adopted from reference (https://spectra.chem.ut.ee/conservation_materials/; accessed and updated on 11 January 2026).

Table 10. Extracted FTIR peaks from Figure 4 used for step-by-step interpretation

No	**Experimental data**			**Wavenumber in reference (cm^{-1})**	**Companion peak(s)**	**Assignment**	**Interpretation role**
	Approx. wavenumber (cm^{-1})	**Peak characteristic**	**Part**				
1	~3085–3026	Sharp, weak–medium	V	3000–3100	Peaks No. 2–4 (aromatic out-of-plane (oop) bending)	Aromatic C–H stretching	Identifies aromatic framework
2	~2949–2871	Sharp, medium	V	2850–2970	Peak No. 1 (aromatic C–H)	Aliphatic C–H stretching	Indicates alkyl substituents
3	~1623–1604	Medium	III	1600–1650	Peaks No. 4–6 (aromatic fingerprint)	Aromatic C=C stretching	Confirms aromatic ring system
4	~1572	Medium	III	1550–1600	Peaks No. 1 & 3	Aromatic skeletal vibration	Supports aromatic structure
5	~1495–1459	Medium	II	1450–1500	Peaks No. 3–4	Aromatic ring vibration	Fingerprint confirmation
6	~1248–1030	Strong	II	1000–1300	Peaks No. 3 & 7	In-plane C–H / ring vibrations	Structural fingerprint
7	~895–692	Sharp, strong	II	690–900	Peaks No. 1 & 3	Aromatic C–H out-of-plane bending	Diagnostic of substituted aromatics
8	~725–345	Sharp, weak	I	300–700	Peaks No. 5–7	Ring deformation/lattice modes	Final structural confirmation

Table 11. Extracted FTIR peaks from Figure 5 used for step-by-step interpretation

No	Experimental data			Wavenumber in reference (cm^{-1})	Companion peak(s)	Assignment	Interpretation role
	Approx. wavenumber (cm^{-1})	Peak characteristic	Part				
1	~3316	Broad, strong	V	3200–3600	Peak No. 2 (1655) for O–H / water correlation	O–H stretching (hydrogen-bonded)	Identifies hydroxyl groups
2	~2973–2881	Sharp, strong	V	2850–2970	Peak No. 4–6 (alkyl bending)	Aliphatic C–H stretching	Indicates alkyl backbone
3	~1655	Medium	III	1600–1650	Peak No. 1 (O–H stretching)	H–O–H bending / O–H deformation	Supports hydrogen bonding
4	~1454–1379	Medium	II	1370–1460	Peak No. 2 (C–H stretching)	CH_2 / CH_3 bending	Alkyl fingerprint confirmation
5	~1327	Medium	II	1300–1350	Peak No. 4	CH_3 symmetric bending	Fingerprint support
6	~1273	Strong	II	1200–1300	Peak No. 1 & 3	C–O stretching	Ether/alcohol confirmation
7	~1087–1045	Very strong	II	1000–1100	Peak No. 6 (C–O stretching)	C–O stretching	Main oxygenated backbone vibration
8	~880	Sharp, weak	II	850–900	Peak No. 2	C–H out-of-plane bending	Structural support
9	~626–431	Weak	I	400–700	Peaks No. 4–8	Skeletal / deformation modes	Final framework confirmation

5.5. Case 5: Aliphatic material

The FTIR spectrum of the representative material is shown in **Figure 6** and is interpreted using the step-by-step workflow based on the master FTIR dataset.

(i) **Step 0. Spectral quality check.** The spectrum spans the full FTIR range (4000–400 cm^{-1}) and exhibits a stable baseline with numerous sharp absorption bands, particularly in the fingerprint region. The spectral quality is sufficient for systematic step-by-step interpretation. The extracted absorption peaks used for analysis are summarized in **Table 12**.

(ii) **Step 1. High-frequency region (PART V, 2500–4000 cm^{-1}).** Strong and sharp absorption bands are observed at approximately 2985, 2916, 2878, and 2833 cm^{-1}, which are characteristic of aliphatic C–H stretching vibrations. A weaker band near 2727 cm^{-1} may be attributed to overtone or combination bands. The absence of broad absorption in the 3200–3600 cm^{-1} region indicates that O–H or N–H groups are not dominant in this material.

(iii) **Step 2. Double-bond region (PART III, 1500–1800 cm^{-1}).** An absorption band is observed at approximately 1644 cm^{-1}. In the absence of strong carbonyl-related peaks near 1700–1750 cm^{-1}, this band is more consistent with C=C stretching or weakly bound water rather than a carbonyl functional group. No prominent ester or ketone carbonyl absorption is detected.

(iv) **Step 3. Triple-bond and cumulative multiple-bond region (PART IV, 1800–2500 cm^{-1}).** No significant absorption bands are observed in this region, excluding the presence of nitrile, alkyne, or related cumulative multiple-bond functionalities.

(v) **Step 4. Fingerprint region (PART II, 700–1500 cm^{-1}).** The fingerprint region contains numerous well-resolved absorption bands. Peaks at approximately 1468, 1445, 1377, and 1365 cm^{-1} are attributed to bending vibrations of alkyl (–CH_2/–CH_3) groups. Strong bands at approximately 1329, 1264, 1220, 1204, 1125, 1100, 1084, 1014, and 974 cm^{-1} are associated with C–C and C–O stretching and deformation modes, indicating a dense aliphatic backbone with multiple substituents.

(vi) **Step 5. Low-frequency region (PART I, 400–700 cm^{-1}).** Distinct absorption bands at approximately 786, 716, 619, 564, 460, 422, 334, and 266 cm^{-1} are observed. These low-frequency features correspond to skeletal deformation and lattice-related modes, providing final supporting evidence for a complex aliphatic organic framework.

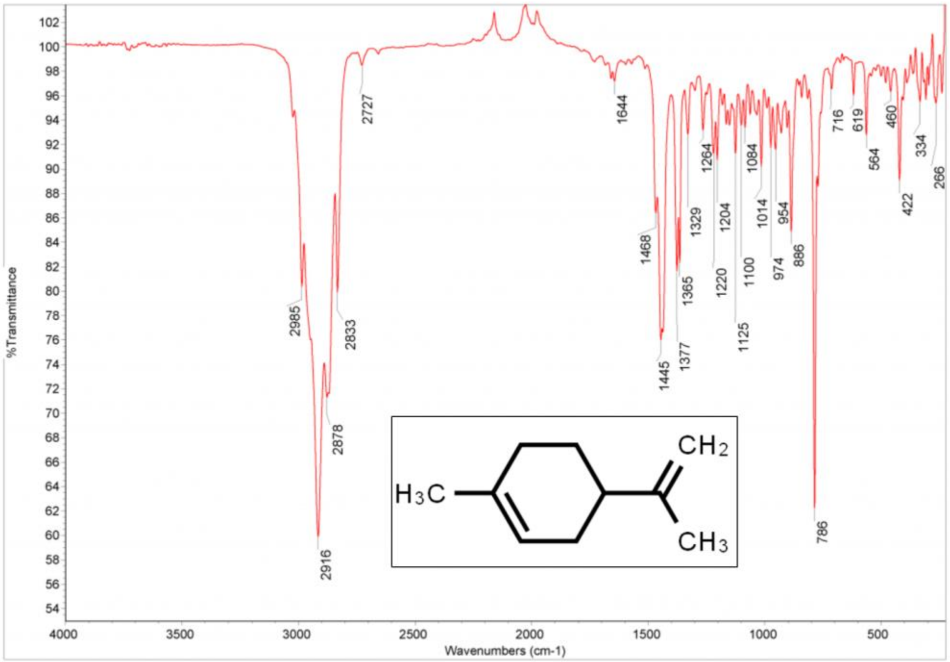

Figure 6. FTIR spectrum of a representative material, Case 5. The figure was adopted from reference (https://spectra.chem.ut.ee/conservation_materials/; accessed and updated on 11 January 2026).

Table 12. Extracted FTIR peaks from Figure 6 used for step-by-step interpretation.

No	Experimental data			Wavenumber in reference (cm^{-1})	Companion peak(s)	Assignment	Interpretation role
	Approx. wavenumber (cm^{-1})	Peak characteristic	Part				
1	~2985–2833	Sharp, strong	V	2850–3000	Peaks No. 4–6 (alkyl bending)	Aliphatic C–H stretching	Identifies aliphatic backbone
2	~2727	Weak	V	2700–2750	Peak No. 1	Overtone / combination band	Minor spectral feature
3	~1644	Medium	III	1600–1650	Peak No. 1 (C–H stretching)	C=C stretching / weak H–O–H bending	Secondary structural indicator
4	~1468–1445	Medium	II	1450–1470	Peak No. 1	CH_2 bending	Alkyl fingerprint confirmation
5	~1377–1365	Medium	II	1360–1380	Peak No. 4	CH_3 bending	Supports alkyl substitution
6	~1329–1204	Strong	II	1200–1350	Peaks No. 1 & 7	C–C / C–O stretching	Main fingerprint backbone
7	~1125–974	Strong	II	950–1150	Peaks No. 6 & 8	Backbone deformation modes	Structural fingerprint
8	~786–266	Sharp, weak	I	250–800	Peaks No. 4–7	Skeletal / lattice modes	Final framework confirmation

5.6. Case 6: Simple polymer

The FTIR spectrum of the representative material is shown in **Figure 7** and is interpreted using the step-by-step workflow based on the master FTIR dataset.

(i) **Step 0. Spectral quality check.** The spectrum spans the full FTIR range (4000–400 cm^{-1}) with a stable baseline and clearly resolved absorption bands. No major artefacts are observed. The extracted absorption peaks used for the step-by-step interpretation are summarized in **Table 13**.

(ii) **Step 1. High-frequency region (PART V, 2500–4000 cm^{-1}).** A broad and intense absorption band is observed at approximately 3276 cm^{-1}, which is characteristic of O–H stretching associated with hydrogen-bonded hydroxyl groups. In addition, distinct absorption bands at approximately 2937 and 2906 cm^{-1} correspond to aliphatic C–H stretching vibrations. The coexistence of O–H and aliphatic C–H features indicates a hydroxyl-containing organic material with an alkyl backbone.

(iii) **Step 2. Double-bond region (PART III, 1500–1800 cm^{-1}).** A strong absorption band is observed at approximately 1709 cm^{-1}, which is characteristic of a carbonyl (C=O) stretching vibration. Additional bands at approximately 1664 and 1560 cm^{-1} are consistent with conjugated C=O/C=C vibrations or amide-like environments. The position and intensity of these bands indicate the presence of a carbonyl-containing functional group, potentially conjugated or hydrogen-bonded.

(iv) **Step 3. Triple-bond and cumulative multiple-bond region (PART IV, 1800–2500 cm^{-1}).** No significant absorption bands are detected in this region, excluding the presence of nitrile, alkyne, or other cumulative multiple-bond functionalities.

(v) **Step 4. Fingerprint region (PART II, 700–1500 cm^{-1}).** The fingerprint region exhibits multiple well-defined absorption bands. Peaks at approximately 1420, 1373, and 1322 cm^{-1} are attributed to bending vibrations of alkyl groups. Strong bands at approximately 1236, 1142, 1085, and 1026 cm^{-1} are associated with C–O stretching vibrations, supporting the presence of ester, ether, or alcohol functionalities. Additional bands at approximately 915 and 839 cm^{-1} correspond to out-of-plane C–H bending modes.

(vi) **Step 5. Low-frequency region (PART I, 400–700 cm^{-1}).** Distinct absorption bands are observed at approximately 548, 474, and 408 cm^{-1}. These low-frequency features are attributed to skeletal deformation and lattice-related modes, providing final supporting evidence for the organic framework.

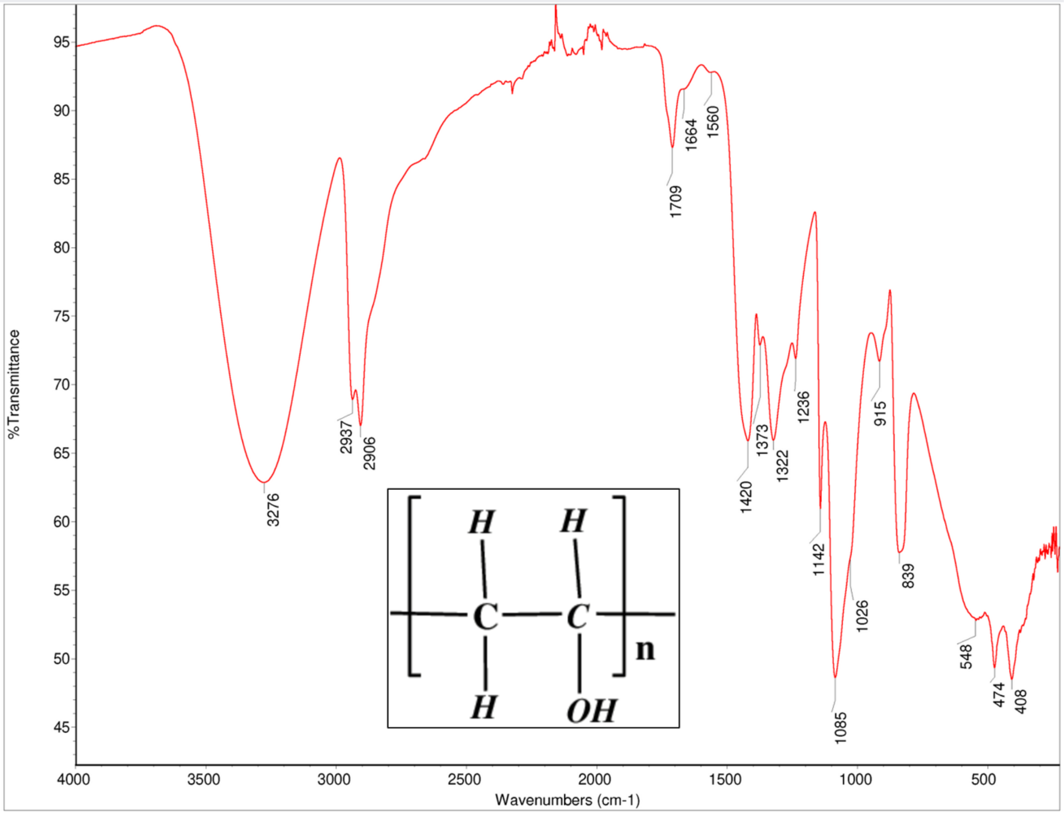

Figure 7. FTIR spectrum of a representative material, Case 6. The figure was adopted from reference (https://spectra.chem.ut.ee/conservation_materials/; accessed and updated on 11 January 2026).

Table 13. Extracted FTIR peaks from Figure 7 used for step-by-step interpretation

No	Approx. wavenumber (cm^{-1})	Peak characteristic	Part	Wavenumber in reference (cm^{-1})	Companion peak(s)	Assignment	Interpretation role
1	~3276	Broad, strong	V	3200–3600	Peak No. 3 (1709)	O–H stretching (hydrogen-bonded)	Identifies hydroxyl groups
2	~2937–2906	Sharp, medium	V	2850–2970	Peaks No. 4–6	Aliphatic C–H stretching	Indicates alkyl backbone
3	~1709	Strong, sharp	III	1700–1750	Peaks No. 1 & 4	C=O stretching	Primary functional group
4	~1664–1560	Medium	III	1550–1650	Peak No. 3	Conjugated C=O / C=C	Supports conjugation
5	~1420–1322	Medium	II	1300–1450	Peak No. 2	CH bending vibrations	Fingerprint alkyl support
6	~1236–1026	Strong	II	1000–1300	Peaks No. 1 & 3	C–O stretching	Oxygenated backbone
7	~915–839	Sharp, weak	II	800–950	Peaks No. 2 & 4	C–H out-of-plane bending	Structural support
8	~548–408	Weak	I	400–700	Peaks No. 5–7	Skeletal deformation modes	Final framework confirmation

5.7. Case 7: Alkyl halide (C–Br, brominated alkyl)

The FTIR spectrum of the representative material is shown in **Figure 8** and is interpreted using the step-by-step workflow based on the master FTIR dataset.

To simplify the interpretation of halogenated organic materials, the analysis in this section focuses only on a limited number of diagnostically significant features rather than exhaustive peak listing. In particular, emphasis is placed on the presence of strong absorption bands in the low-frequency region (PART I, 400–700 cm^{-1}), which play a decisive role in distinguishing alkyl halides from non-halogenated aliphatic compounds.

(i) **Step 0. Spectral quality check.** The spectrum covers the full FTIR range (4000–400 cm^{-1}) with a stable baseline and clearly resolved absorption bands. The spectrum quality is adequate for systematic interpretation. The extracted absorption peaks used for the step-by-step analysis are summarized in **Table 14**.

(ii) **Step 1. High-frequency region (PART V, 2500–4000 cm^{-1}).** Strong absorption bands are observed at approximately 2976 and 2940 cm^{-1}, which correspond to aliphatic C–H stretching vibrations. No absorption bands are present above 3000 cm^{-1}, indicating the absence of aromatic or olefinic C–H groups. In addition, no broad O–H or N–H stretching bands are detected in the 3200–3600 cm^{-1} region.

(iii) **Step 2. Double-bond region (PART III, 1500–1800 cm^{-1}).** No strong absorption bands characteristic of carbonyl (C=O) or C=C stretching are observed in this region. This indicates that double-bond functionalities are not present in the molecular structure.

(iv) **Step 3. Triple-bond and cumulative multiple-bond region (PART IV, 1800–2500 cm^{-1}).** No diagnostic absorption bands are detected in the triple-bond region, excluding the presence of nitrile, alkyne, or cumulative multiple-bond groups.

(v) **Step 4. Fingerprint region (PART II, 700–1500 cm^{-1}).** Distinct absorption bands are observed at approximately 1291 and 1230 cm^{-1}. These bands are assigned to C–H wagging vibrations, which are commonly associated with terminal alkyl halides (–CH_2X). This fingerprint feature is particularly important because it helps differentiate alkyl halides from non-halogenated alkanes.

(vi) **Step 5. Low-frequency region (PART I, 400–700 cm^{-1}).** A strong absorption band is observed at approximately 651 cm^{-1}, which is characteristic of C–Br stretching vibrations. The presence of this low-frequency band provides direct and definitive evidence for a brominated alkyl structure.

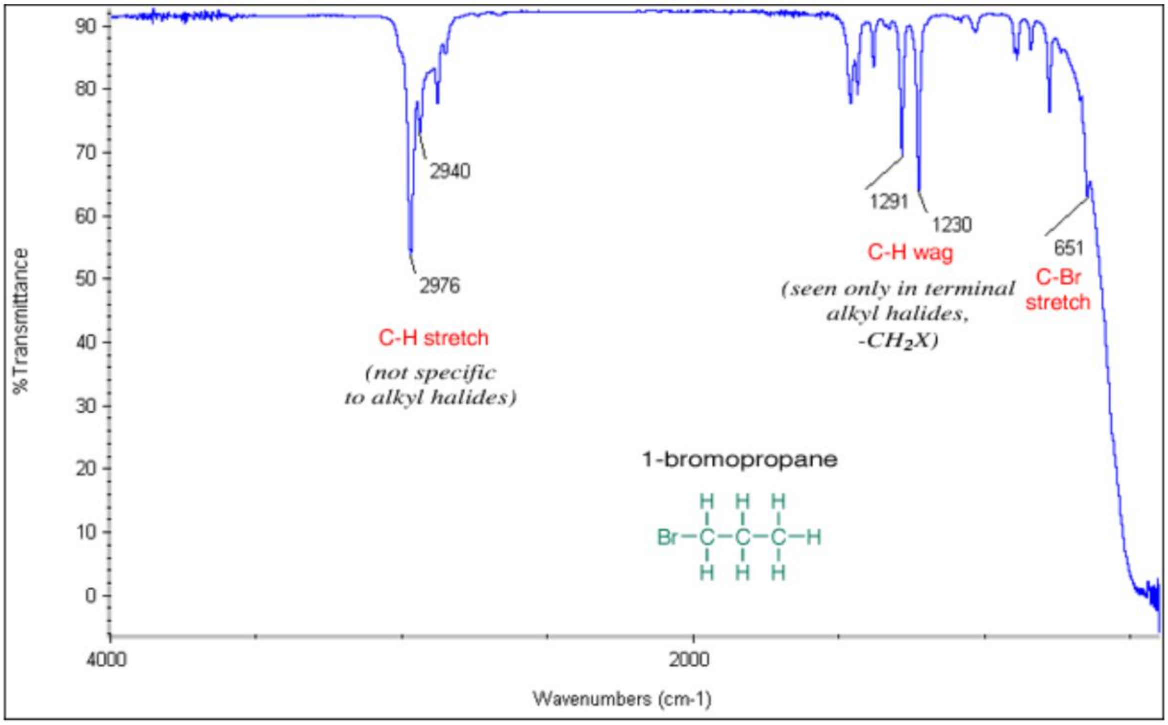

Figure 8. FTIR spectrum of a representative material, Case 7. The figure was adopted from reference (https://orgchemboulder.com/Spectroscopy/irtutor/alkhalidesir.shtml; accessed and updated on 11 January 2026).

Table 14. Extracted FTIR peaks from Figure 8 used for step-by-step interpretation

No	Approx. wavenumber (cm^{-1})	Peak characteristic	Part	Wavenumber in reference (cm^{-1})	Companion peak(s)	Assignment	Interpretation role
1	~2976–2940	Sharp, strong	V	2850–3000	Peak No. 3–4 (alkyl bending/wagging)	Aliphatic C–H stretching	Identifies alkyl backbone
2	~1291	Medium	II	1250–1350	Peak No. 5 (C–Br stretching)	C–H wagging (–CH_2X)	Diagnostic for alkyl halide
3	~1230	Medium	II	1200–1300	Peak No. 5 (C–Br stretching)	C–H wagging (–CH_2X)	Supports terminal halogen substitution
4	~651	Strong, sharp	I	600–700	Peaks No. 2–3 (CH wagging)	C–Br stretching	Direct identification of brominated alkyl
5	–	–	III/IV	–	Absence of C=O / C≡N	–	Excludes carbonyl and multiple-bond groups

5.8. Case 8: Alkyl halide (C–Cl, chlorinated alkyl)

The FTIR spectrum of the representative material is shown in **Figure 9** and is interpreted using the step-by-step workflow based on the master FTIR dataset. To simplify the interpretation of halogenated organic materials, the analysis in this section focuses only on a limited number of diagnostically significant features rather than exhaustive peak listing. In particular, emphasis is placed on the presence of strong absorption bands in the low-frequency region (PART I, 400–700 cm^{-1}), which play a decisive role in distinguishing alkyl halides from non-halogenated aliphatic compounds.

(i) **Step 0. Spectral quality check.** The spectrum covers the full FTIR range (4000–400 cm^{-1}) with a stable baseline and clearly resolved absorption bands. No significant artefacts are observed, indicating that the spectrum is suitable for systematic interpretation. The extracted absorption peaks used for the step-by-step analysis are summarized in **Table 15**.

(ii) **Step 1. High-frequency region (PART V, 2500–4000 cm^{-1}).** Strong absorption bands are observed at approximately 2976 and 2873 cm^{-1}, which correspond to aliphatic C–H stretching vibrations. No absorption is detected above 3000 cm^{-1}, indicating the absence of aromatic or olefinic C–H groups. In addition, no broad bands are present in the 3200–3600 cm^{-1} region, excluding O–H or N–H functionalities.

(iii) **Step 2. Double-bond region (PART III, 1500–1800 cm^{-1}).** No strong absorption bands characteristic of carbonyl (C=O) or C=C stretching are observed in this region. This confirms the absence of double-bond-containing functional groups.

(iv) **Step 3. Triple-bond and cumulative multiple-bond region (PART IV, 1800–2500 cm^{-1}).** No diagnostic absorption bands are detected in this region, excluding nitrile, alkyne, or cumulative multiple-bond functionalities.

(v) **Step 4. Fingerprint region (PART II, 700–1500 cm^{-1}).** A characteristic absorption band is observed at approximately 1271 cm^{-1}, which is assigned to C–H wagging vibrations associated with terminal alkyl halides (–CH_2X). This band serves as an important fingerprint feature for identifying halogenated alkyl chains.

(vi) **Step 5. Low-frequency region (PART I, 400–700 cm^{-1}).** Distinct absorption bands are observed at approximately 743 and 687 cm^{-1}. These bands are characteristic of C–Cl stretching vibrations. The presence of these low-frequency bands provides definitive evidence for a chlorinated alkyl structure.

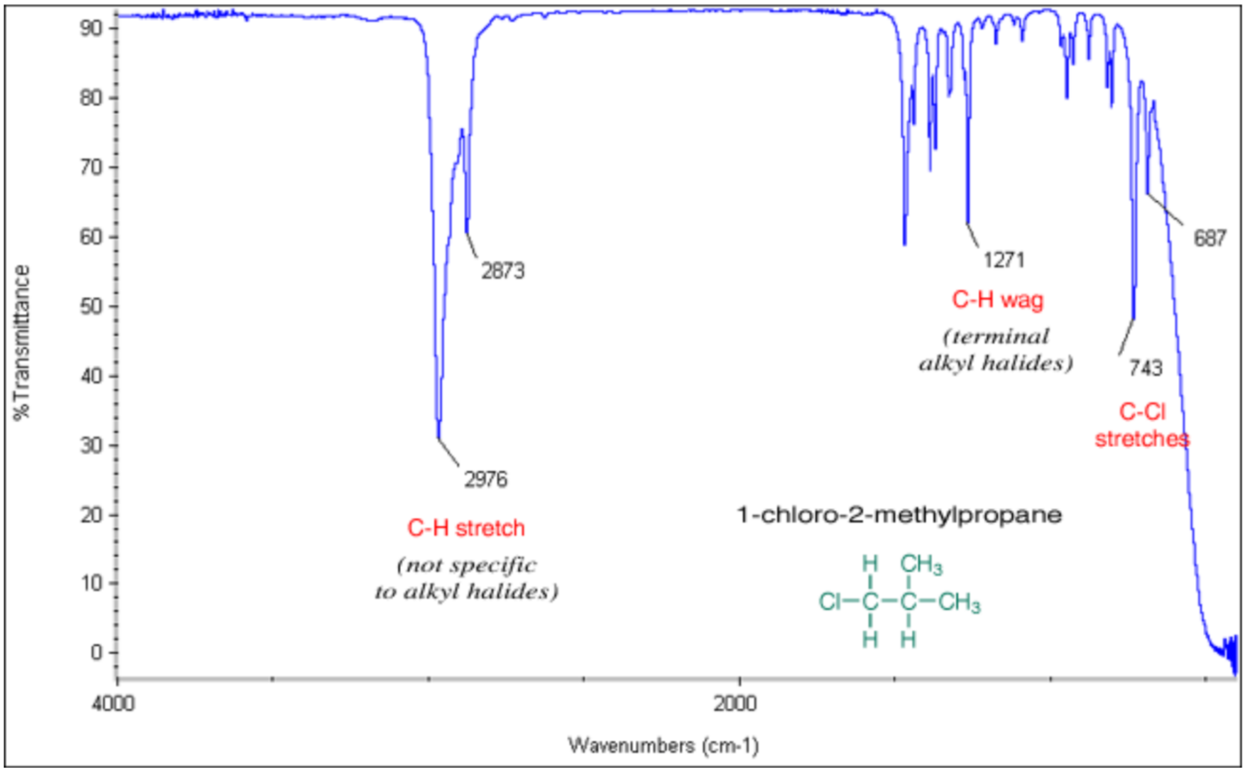

Figure 9. FTIR spectrum of a representative material, Case 8. The figure was adopted from reference (https://orgchemboulder.com/Spectroscopy/irtutor/alkhalidesir.shtml; accessed and updated on 11 January 2026).

Table 15. Extracted FTIR peaks from Figure 9 used for step-by-step interpretation

No	Approx. wavenumber (cm⁻¹)	Peak characteristic	Part	Wavenumber in reference (cm⁻¹)	Companion peak(s)	Assignment	Interpretation role
1	~2976–2873	Sharp, strong	V	2850–3000	Peak No. 3 (C–H wagging)	Aliphatic C–H stretching	Identifies alkyl backbone
2	~1271	Medium	II	1250–1350	Peak No. 4–5 (C–Cl stretching)	C–H wagging (–CH_2X)	Diagnostic for alkyl halide
3	~743	Strong, sharp	I	700–800	Peak No. 2 (C–H wagging)	C–Cl stretching	Primary evidence of chlorination
4	~687	Medium	I	600–700	Peak No. 2	C–Cl stretching	Supporting halogen confirmation
5	–	–	III/IV	–	Absence of C=O / C≡N	–	Excludes multiple-bond groups

6. FUTURE PERSPECTIVE: INTEGRATION WITH DATA-DRIVEN AND AI-BASED ANALYSIS

The master FTIR dataset developed in this study is not limited to manual or expert-based interpretation. Its structured organization into spectral regions, functional group classifications, peak characteristics, and correlated peak families makes it directly suitable for integration into data-driven frameworks. Such structured datasets are essential prerequisites for the development of AI and ML models for automated FTIR interpretation.

The step-by-step workflow presented in this work can serve as a rule-based foundation for feature extraction, labeling, and training dataset construction. Peak families and correlation rules can be translated into supervised learning labels, while spectral regions can be used to guide region-specific feature engineering. This approach is particularly relevant for polymer systems, composite materials, and hybrid organic–inorganic structures, where conventional peak-matching algorithms often fail.

In future applications, the master dataset may support the development of intelligent FTIR systems capable of automated functional group identification, material classification, and anomaly detection. Integration with AI and ML tools has the potential to enhance reproducibility, reduce operator dependency, and accelerate materials screening in chemical engineering, materials science, and particle technology. Therefore, the dataset presented in this study provides not only an interpretative guide but also a foundational resource for next-generation FTIR analysis platforms.

7. CONCLUSION

This study introduces a master FTIR dataset integrated with a step-by-step peak-correlation workflow to improve the clarity, consistency, and reliability of FTIR spectrum interpretation. By organizing FTIR information into five spectral regions and emphasizing correlated peak families rather than isolated bands, the proposed approach reduces misinterpretation, particularly for complex materials such as polymers, blends, and functionalized systems. Representative case studies demonstrate the applicability of the method across a wide range of materials. Importantly, the structured nature of the dataset enables future extension toward data-driven and artificial intelligence-based FTIR analysis. As such, this work serves not only as a practical guide for manual interpretation and education but also as a foundational dataset for the development of automated and intelligent materials characterization tools.

8. AUTHORS' NOTE

The authors declare that there is no conflict of interest regarding the publication of this article. Authors confirmed that the paper was free of plagiarism.

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