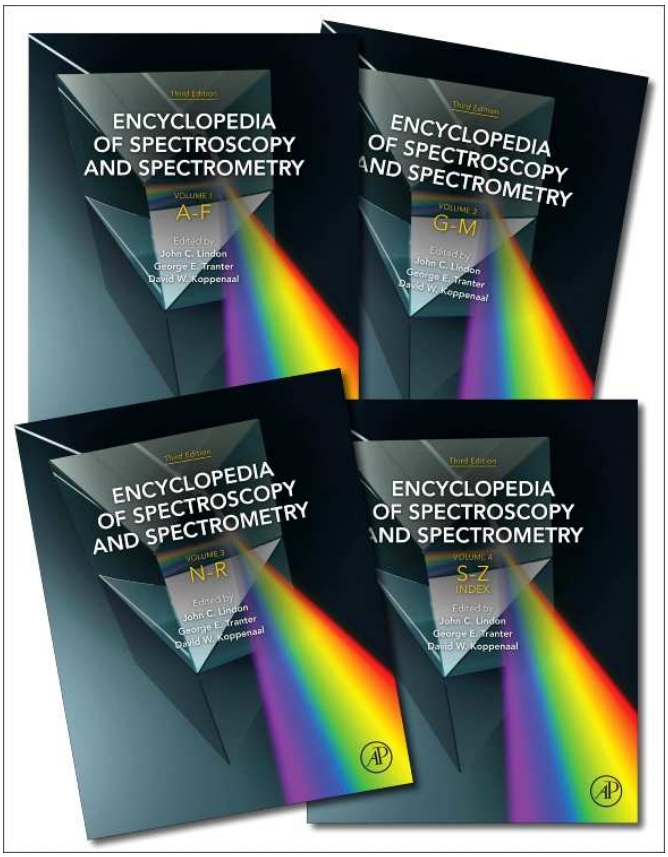

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IR Spectroscopy, Soil Analysis Applications

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Introduction

Fourier transform infrared (FTIR) spectroscopy is a unique tool for the study of mineral and organic components of soil samples. FTIR spectroscopy offers sensitive characterization of minerals and soil organic matter (SOM), and mechanistic and kinetic aspects of mineral–SOM interactions that underlie biogeochemical processes. The molecular resolution of mineral and organic functional groups provided by FTIR has contributed significantly to understanding mineral and SOM structures, and ion and organic molecule sorption to mineral surfaces. The versatility of FTIR spectroscopy makes it a foundational tool for soil scientists, despite challenges in the acquisition and interpretation of soil spectra that stem from chemical heterogeneity. Recent advances in acquisition methods increasingly enable resolution of in situ compositional and temporal complexity of the soil milieu and chemical reactions occurring in this complex matrix.

FTIR Sampling Techniques for Soils

Soil samples can be analyzed by FTIR spectroscopy using a variety of methods, the most common of which are transmission, diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS), and attenuated total reflectance (ATR). Different modes of acquiring FTIR spectra offer complementary methods for evaluating soil components and processes. *Transmission spectroscopy* was the earliest method used to collect FTIR spectra of soil mineral and organic components. Soil extracts (eg, NaOH-extractable SOM) or suspensions are dried onto infrared (IR) windows (eg, ZnSe, Ge) prior to analysis, and solid samples such as soils or SOM fractions are ground, mixed, and diluted with potassium bromide (KBr; 0.5–3% sample), pressed into pellets, and dessicated prior to analysis. Transmission provides a bulk IR measurement because the beam encounters all parts of the sample, which is in contrast to other collection methods such as ATR. Due to the labor of sample preparation and artifacts that can be introduced upon pellet desiccation, transmission spectroscopy is used less frequently today and less labor-intensive methods have gained favor.

One such method is DRIFTS, which entails minimal sample preparation (eg, drying and grinding). Soil samples should be uniformly and finely ground (<900 μm) to avoid artifacts and further homogenize samples. In unground samples, artifacts may arise due to coarser particle sizes trapping light more effectively than finer particle sizes which can increase IR scattering. This can result in higher absorbance and a shifted baseline, altered peak widths, and non-linear absorbance. DRIFTS can be performed on undiluted "neat" soil samples, or using KBr dilution of soil samples (2–10% sample). The suitability of KBr dilution is assessed empirically to determine if spectral quality is improved, or as a necessity when only small sample volumes are available (Fig. 1).

The most recent FTIR technique for soil analysis is *attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR)*, unique in that it offers in situ study of soil minerals, SOM, bacteria, and other samples in the presence of water. ATR-FTIR spectra provide information on functional groups near the surface (~1 μm) of an internal reflection element (IRE). A key advantage to ATR-FTIR relative to other FTIR collection methods, and analytic techniques in general, is the ability to collect accurate spectra of samples in the presence of water. Water absorbs strongly in the mid-IR range where the absorbance of soil components also occurs (eg, 3300, 1640 cm^{-1}); thus, limiting the application of transmission and DRIFTS analyses to desiccated samples. However, ATR-FTIR has been successfully used to resolve soil processes occurring in aqueous conditions and at surface–liquid interfaces, including:

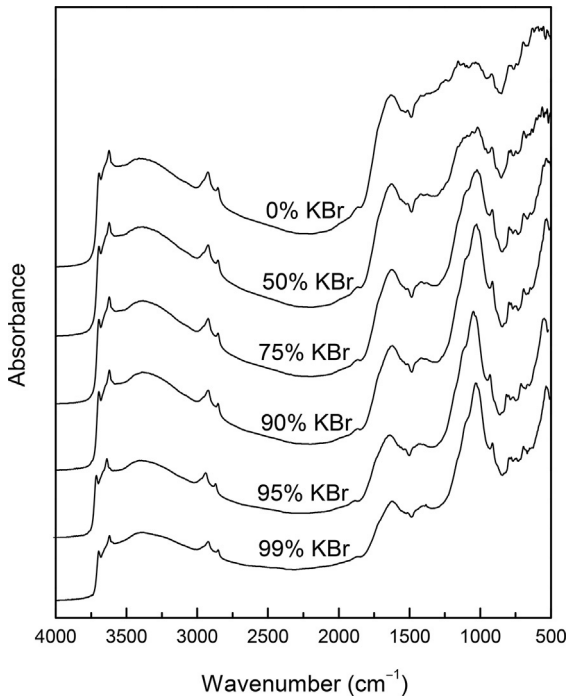

Fig. 1 Diffuse reflectance infrared Fourier transform spectra of a high organic matter soil (120 g C kg^{-1} soil) across a range of KBr dilution.

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(1) Sorption of aqueous species at crystal and mineral-coated crystal interfaces to provide information on the speciation of bound molecules and differentiate between inner- and outer-sphere surface complexes.
(2) Interactions at the bacteria-mineral and biomolecule-mineral interface to elucidate biomolecule reactions with inorganic solids.

Soil Mineral Analysis

FTIR spectroscopy is a versatile tool for characterizing soil mineral components, including mineral identification, structural assessment, and in situ monitoring of pedogenic processes (e.g., mineral formation). FTIR spectroscopy complements other analytical techniques, most notably X-ray diffraction (XRD) used for mineral identification. Specific absorption fingerprints are sufficiently sensitive to distinguish among shared bond types (e.g., Si—O, Al—O) by the local structural environment, thus enabling soil mineral identification and characterization.

Phyllosilicates

Phyllosilicates are the most common class of soil minerals. Also known as layer silicates, these minerals consist of (i) Al in octahedral coordination with O(H) that are bound to (ii) one (1:1) or two (2:1) sheets of Si in tetrahedral coordination with O. The sensitivity of IR absorbance to these bond types, their coordination, and other characteristics of the mineral structure (e.g., isomorphic substitution, interlayer cations, and crystallinity) enable identification of phyllosilicate structural class (1:1 vs. 2:1 layer silicates) and specific mineral types within each structural class (e.g., kaolinite vs. nacrite), as well as structural details (e.g., di- vs. trioctahedral) and compositional information (e.g., interlayer cations).

Phyllosilicate identification and structural characterization is based on absorbances by mineral structural units, most notably hydroxyl, silicate, and interlayer and octahedral layer cations. Hydroxyl O—H stretching and bending occur at 3750–3400 cm^{-1} and 950–600 cm^{-1}, respectively (Fig. 2). Silicate Si—O stretching occurs at 1200–700 cm^{-1} and 700–400 cm^{-1}, potentially overlapping with octahedral cation absorbances in the latter range. In contrast, interlayer cations produce absorbance bands outside the mid-IR range, in far-IR (150–70 cm^{-1}).

The 2:1 layer silicates contain a single OH stretching band 3700–3620 cm^{-1}, whereas 1:1 layer silicates exhibit two or more OH stretching bands in this region. The number and location of bands in this range are sufficiently sensitive to mineral structure to differentiate minerals within each layer silicates class. For 1:1 layer silicates, absorbance at 3630–3620 cm^{-1} reflects internal OH groups between the tetrahedral and octahedral sheets, and absorbance at 3700 cm^{-1} reflects internal H-bonding between octahedral surface OH and O from the underlying tetrahedral layer. In 2:1 layer silicates, isomorphic substitution disrupts crystalline order, causes the single band at 3700 cm^{-1} to be broad, and its precise wavenumber will vary depending on the cation(s) to which tetrahedral layer OH are bonded.

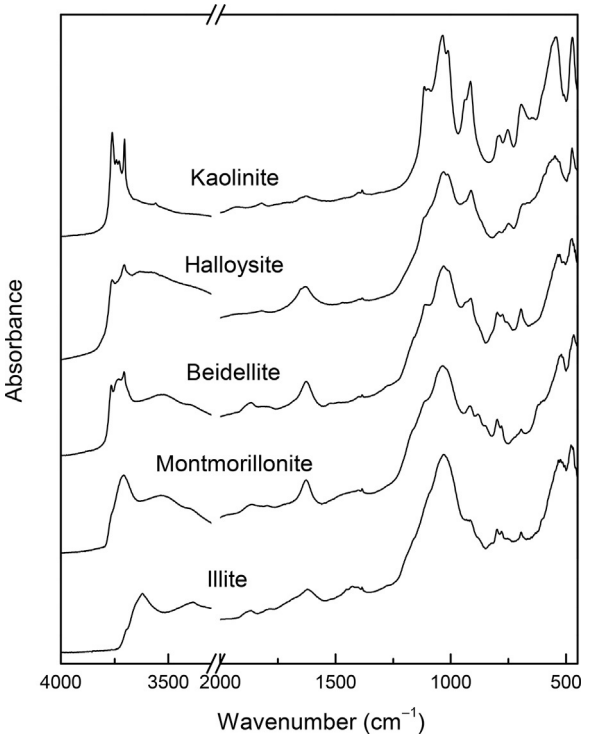

Fig. 2 Diffuse reflectance infrared Fourier transform spectra of 1:1 (kaolinite, halloysite) and 2:1 (beidellite, montmorillonite, and illite) layer silicates diluted (5%) in KBr.

The Si—O stretch and OH bend region is useful for identifying layer silicates class. The 1:1 layer silicates express a triumvirate of Si—O absorbances at 1120–950 cm^{-1}, whereas the 2:1 layer silicates exhibit a single broad absorbance peak at 1030–1010 cm^{-1}. Furthermore, such Si—O stretch bands occur at higher wavenumbers for trioctahedral minerals (1030–1020 cm^{-1}) than for dioctahedral minerals (~1010 cm^{-1}). Absorbance bands from OH bending in di- and trioctahedral 1:1 layer silicates occur at 950–800 cm^{-1} and 700–600 cm^{-1}, respectively. In 2:1 layer silicates, OH bending absorbances occur 950–915 cm^{-1} and can reflect octahedral cation composition, such as MgAlOH at 840 cm^{-1} in montmorillonite.

Allophane and Imogolite

Allophane and imogolite are hydrated aluminosilicate minerals exhibiting short-range order crystallinity. These minerals can strongly influence soil chemical processes due to their high surface area and reactivity, and are common in soil orders of Andisols and Spodosols. FTIR spectroscopy can be used to distinguish among allophane and imogolite in soils by O—H stretching (3800–2800 cm^{-1}) and deformation (1700–1550 cm^{-1}), and Si—O stretching (1200–800 cm^{-1}), and Si—O bending at 348 cm^{-1} can be used to (semi-)quantify these minerals.

Metal Oxides, Hydroxides, and Oxyhydroxides

FTIR spectroscopy enables the identification and characterization of metal oxides, a mineral class common in soils that includes oxides, hydroxides, and oxyhydroxides of metals such as iron, aluminium, and manganese. FTIR spectroscopy can be used to characterize and study both crystalline and poorly crystalline metal oxides, thus providing a distinct advantage over XRD, which is primarily limited to crystalline samples.

The O—H stretch is highly sensitive to oxide type and properties (e.g., crystallinity, specific conformation of polymorph), and consequently these absorbance bands can be used to identify and determine metal oxide type, structure, and properties. For example, O—H stretch bands for gibbsite ($Al(OH)_3$; Fig. 3), the most common Al oxide in soils, exhibit a number of bands and band frequencies reflecting the degree of crystallinity.

Goethite (α-FeOOH) and hematite (α-Fe_2O_3) are two common iron oxides found in soil; other Fe oxides present in soils include ferrihydrite, lepidocrocite, maghemite, magnetite, and schwertmannite. These metal oxides are key indicators of pedogenic processes such as weathering, and strongly influence soil color and the retention of ions, SOM, and anthropogenic compounds. FTIR has proven to be a key tool for identifying and characterizing these mineral species, particularly for non-crystalline forms that are not readily characterized by other methods. Fe—O and FeO—H absorbances can be used to identify the type of Fe oxide or polymorph, and determine crystallinity and cation substitution. Differences in the coordination of Fe with O result in specific Fe—O and FeO—H absorbances at 3400–3000 cm^{-1}, 900–700 cm^{-1}, and <700 cm^{-1} (Fig. 3). Absorbance bands of O—H stretching and bending reflect the degree of cation substitution. For example, increasing Al substitution in goethite manifests as an increase in wavenumber and band broadening for O—H stretching at 3153 cm^{-1}, and in-plane and out-of-plane O—H deformation at 839 cm^{-1} and 894 cm^{-1}. Band broadening can also reflect decreasing crystallinity.

Mineral Weathering and Pedogenesis

The monitoring of soil weathering reactions and pedogenesis, such as chemical alteration of mineral surfaces and the formation of new mineral phases, is possible using FTIR. FTIR spectroscopy offers characterization of structural and kinetic aspects of biogeochemical processes that are not otherwise possible in mixed, complex systems, nor possible at the spatial or temporal scale of traditional field approaches employed in soil science. A number of studies have used FTIR for rapid data acquisition that can aid in explaining mineral weathering characterized by XRD. Advantages of FTIR over XRD include the greater speed to temporally resolve reactions and the identification of non-crystalline and amorphous minerals. Finally, the in situ capabilities of FTIR facilitate monitoring of mineral weathering and formation. For example, in in situ techniques such as flow-cell ATR-FTIR can be used to monitor biogenic Mn oxide formation on bacteria biofilms.

SOM Analysis

FTIR spectroscopy is strongly suitable for characterizing organic matter (OM) in soil samples. The functional groups in OM that express dipole moments, and are therefore IR absorbing, strongly influence SOM properties. The presence of O, N, and S functional groups provides SOM with its high chemical reactivity (e.g., cation-exchange capacity, sorption of metals), and a number of functional groups reflect larger structural units such as proteins and polysaccharides related to the nutrient functions and stabilization of SOM. Fortuitously, the carboxyl group (C═O) which modulates a number of SOM

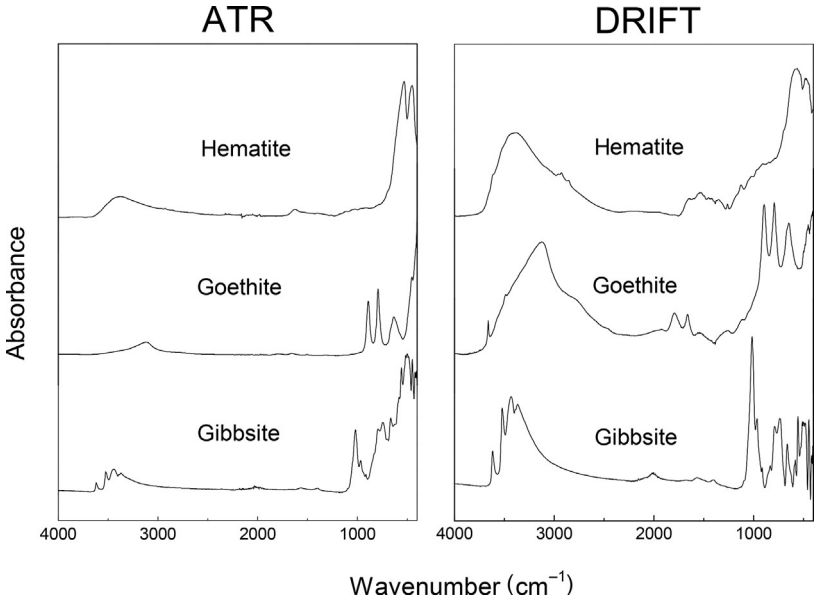

Fig. 3 Comparison of spectra of metal oxides obtained by attenuated total reflectance (ATR) and diffuse reflectance infrared Fourier transform (DRIFT) methods.

properties is highly sensitive to local structural environments and can be well-characterized by FTIR spectroscopy.

Application of FTIR spectroscopy to soil requires compromises and faces limitations specific to the sample type. In contrast to single compounds or simple, known mixtures, SOM is a complex and heterogeneous mixture of functional groups, thus requiring soil-specific FTIR methodologies and data interpretation. The major limitation of FTIR for SOM analysis arises from mineral dominance and absorbance interference. Sample selection and preparation, and/or spectra treatment are key strategies for overcoming this challenge. It is important to note that other analytic approaches to SOM have their own limitations, many of which also originate from the mineral component of soil samples, including nuclear magnetic resonance (NMR) spectroscopy and pyrolysis mass spectrometry.

In the majority of agricultural soils, organic matter makes up a small part of the soil (often less than 5% by weight) with the rest being minerals, largely sand and clays. The relatively low SOM content co-occurs with dominance and overlap of mineral absorbances, in particular Si—O bands, challenging assignments of mineral and organic functional groups. These issues can be addressed by three experimental approaches, with differing trade-offs: (i) employing whole soil samples with limited OM absorbance and interpretation; (ii) soil fractions or extracts enriched in OM; and (iii) calculation of subtraction or difference spectra, in which a spectrum of SOM is obtained indirectly by subtraction of samples that have undergone SOM removal (e.g., combustion, oxidation).

SOM Analysis in Whole Soils

In contrast with the analysis of soil fractions or extracts, DRIFTS analysis of whole soil samples involves minimal to no sample preparation, and can allow for semi-quantitative assessments of bulk SOM. Furthermore, additional data on the soil matrix (e.g., soil mineralogy) is obtained. Controlling for mineral absorbances by comparing bands within the same soil spectrum can be used to highlight differences in absorbances attributable to SOM (Fig. 4). Specific ratios of organic bands in whole soil spectra have been successfully used to characterize SOM or its influence on soil properties. For example, the ratio of band intensity or area for aliphatic C—H stretching at 3000–2800 cm^{-1} relative to carbonyl C═O stretching at 1740–1600 cm^{-1} can provide a measure of soil hydrophobicity that corresponds to soil wettability. The ratio of aliphatic C—H stretching at 3000–2800 cm^{-1} relative to aromatic C═C stretching and/or amide C═O stretching at 1660–1580 has been used as an index of SOM humification.

However, meaningful quantification of many SOM absorbances is generally challenged by low absorbance intensity of organic functional groups relative to the dominant absorbance of mineral components, in particular Si—O stretching at 1100–950 cm^{-1}. Substantial overlap of organic and mineral absorbances can occur in the range 1400–800 cm^{-1}, making difficult unambiguous assignments.

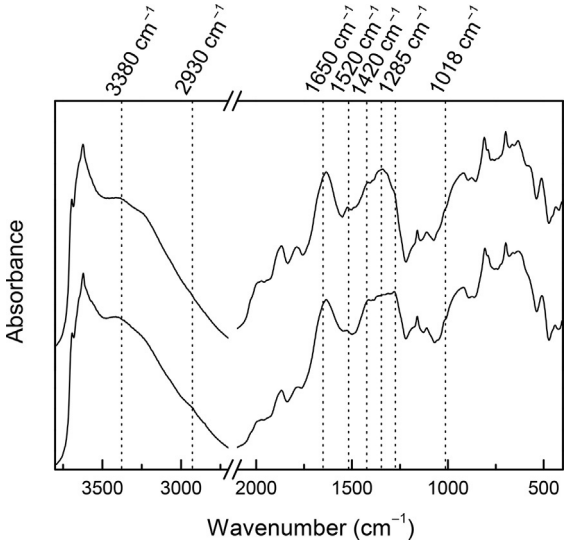

Fig. 4 Diffuse reflectance infrared Fourier transform (DRIFT) spectra of two surface soils of the same mineralogy under agricultural use that contain low and high SOM content (top, 20.7 g C kg^{-1} soil; bottom, 6.2 g C kg^{-1} soil), collected without KBr dilution. Absorbance bands corresponding to organic functional groups are indicated, including amide N—H and alcohol O—H (3380 cm^{-1}), aliphatic C—H (2930, 1420 cm^{-1}), aromatic C═C and/or amide C═O (1650 cm^{-1}), amide C—N and/or aromatic C═C (1520 cm^{-1}), phenol and/or carboxyl C—O (1280 cm^{-1}), and polysaccharide C—O (1018 cm^{-1}). Varying overlap of mineral absorbances with these bands challenges quantification of organic functional groups.

SOM Analysis via Fractions and Extracts

SOM fractions (chemical and physical) and extracts are generally enriched in SOM relative to the bulk soil from which they are obtained, resulting in greater detection of organic absorbances. While this limits analysis to a portion of the total SOM pool, the FTIR analysis of SOM fractions or extracts is useful for studying the conceptual model of the total SOM pool as the composite of smaller pools defined by fractionation and extraction. In particular, FTIR spectroscopy offers molecular-scale resolution of fractions and extracts, extending their utility beyond mass balance values and potentially increasing sensitivity of these fractions to environmental factors influencing SOM such as land use and climate. Common chemical fractions and extracts include particle size fractions, dissolved organic matter or water-extractable organic matter, pyrophosphate-extractable organic matter, and NaOH-extractable organic matter (humic substances). For FTIR transmission and DRIFT analyses, extracts must be lyophilized to minimize water interference.

Physical fractions of soil are obtained by gravimetric and aggregate size properties, and are well-established techniques used in soil science to gain insight on SOM stabilization and turnover. The FTIR analysis of physical fractions strongly complements mass balance approaches to organo-mineral interactions, which are often not detectable in bulk soils (Fig. 5). Such fractions, in particular aggregates, are well suited for FTIR characterization for reasons that are both practical (i.e., no additional sample preparation, enriched in OM) and

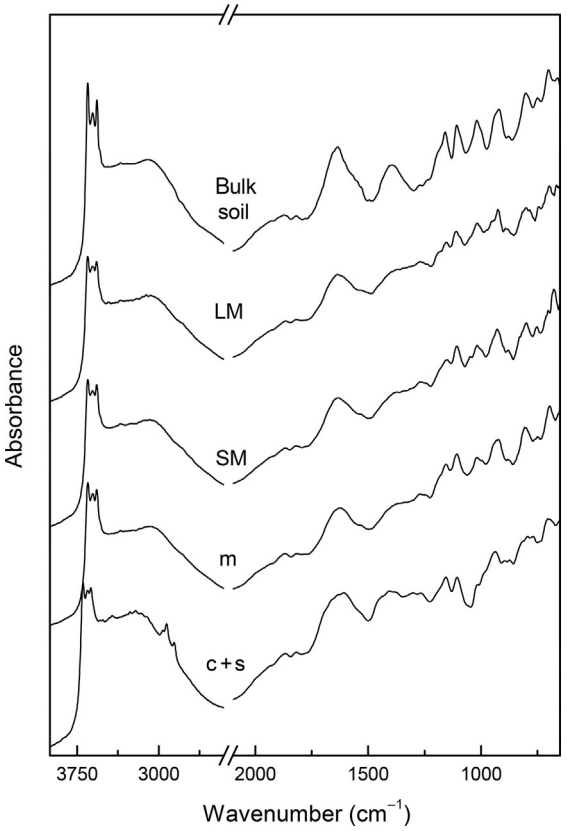

Fig. 5 Diffuse reflectance infrared Fourier transform spectra of a bulk soil and soil physical size fractions: large macroaggregates (LM; 4000–2000 μm), small macroaggregates (SM; 2000–250 μm), microaggregates (m; 250–53 μm), and clay + silt (c + s; <53 μm). Spectra were collected on KBr diluted samples (2%).

theoretical (mechanisms of SOM stabilization implicate differences in composition detectable by FTIR spectroscopy).

SOM Analysis via Removal of Mineral Absorbances

An indirect strategy to improve detection of OM absorbances in soil samples is to enhance absorbance bands by mathematically removing interfering mineral absorbances (i.e., spectral subtraction). The background or subtracted spectrum is most appropriately obtained by treating the sample to remove SOM (e.g., ashing and oxidation). In model soil systems, a pure mineral standard can be used. Alteration of the mineral or organic component during treatments to obtain background samples can produce artifacts in the subsequent subtraction that compromise the utility of subtraction spectra. Whether or not these artifacts present a challenge for interpretation depends on experimental objectives and understanding of specific artifacts, including how and where in the spectrum artifacts manifest. For example, ashing soil to remove SOM can alter mineral absorbances via phyllosilicate dehydration, collapse, and dehydroxylation. However, soil analyses in which discrimination among soils is the objective, rather than characterizing SOM composition, mineral-specific ashing artifacts in subtraction spectra may in fact improve sensitivity of spectral soil fingerprints. Monitoring mineral absorbance bands sensitive to thermal alteration across ashing treatments is an empirical approach to avoid or account for subtraction artifacts. Currently, alternative methods are being explored for SOM removal with minimal collateral damage to minerals and consequentially insignificant, spectroscopically minimal, or well-defined artifacts in subtraction spectra, most notably chemical oxidation (e.g., hydrogen peroxide, sodium hypochlorite). Hydrofluoric acid (HF) can also be used to demineralize soils and is a common pretreatment for other analyses such as NMR. However, SOM removal and compositional alteration during HF treatment may compromise accuracy of structural characterizations, including FTIR spectroscopy.

Monitoring Molecular-Scale Interactions at Solid–Liquid Interfaces

Mineral surfaces are hotspots of chemical and physical processes underlying many soil processes. Molecules that encounter and react with mineral surfaces can be involved in a number of processes such as sorption–desorption, surface complexation, oxidation reduction, and polymerization, with implications for mineral dissolution and formation, SOM stabilization and turnover, and contaminant transport and fate. The in situ analytical capacity of FTIR spectroscopy coupled with its sensitivity to both mineral and organic bonds makes it an ideal tool for monitoring and characterizing the solid–liquid interface. The development of ATR-FTIR in the late 1990s made possible the study of mineral surface reactions because (i) mineral coatings can be created on the IRE and (ii) accurate spectra can be obtained in the presence of water. In contrast, transmission and DRIFTS methods generally produce poor spectra for aqueous samples, and desiccation of samples may lead to artifacts due to dehydration effects and associated changes in pH on molecule–mineral interactions.

Organic Molecular Interactions With Mineral Surfaces

FTIR spectroscopy enables rapid and sensitive analysis of changes in the molecular structure of an adsorbed species (adsorbate) bound to an adsorbent relative to its unbound, aqueous counterpart (adsorptive), as well as molecular changes in the adsorbent as a function of binding. The ability of FTIR to resolve inner- and outer-sphere complex formation on mineral surfaces and the types of surface complex structures formed have improved understanding of sorption processes in soils. There are three common coordination modes in the structural complexes formed by a carboxylate group with a cation at the mineral surface: (1) monodentate binding; (2) chelating bidentate; and (3) bridging bidentate. The formation of these coordination modes can be distinguished through determination of the separation distance (cm^{-1}) between the asymmetric and symmetric COO^- stretching vibrations ($\Delta\nu = \nu_{as}COO^- - \nu_s COO^-$).

The pioneering work by Tejedor-Tejedor and coworkers demonstrated how in situ analysis of organic molecules could be carried out using ATR-FTIR to elucidate sorption mechanisms to mineral surfaces. To avoid interference from a heterogeneous background matrix (SOM and various minerals), research on binding mechanisms of small organic molecules

in soil samples has been conducted using pure mineral phases such as metal oxides and phyllosilicates.

FTIR spectroscopy has been used considerably to evaluate the interactions of agrochemicals and contaminants with layer silicates and metal oxides. Elucidating mechanisms of adsorption between such compounds and minerals is valuable for determining chemical fate and transport in the environment, particularly in subsoil horizons where organic carbon content is generally minimal. Additionally, drivers of binding strength such as interlayer cation-carboxyl interactions can be identified and characterized across a range of conditions. To this end, FTIR, in particular in situ techniques such as ATR-FTIR, can be used to simultaneously determine binding quantitatively and the chemical nature of such binding (e.g., conformations, bond formation). Reactions of herbicides (e.g., 2,4-dichlorophenoxyacetic acid) and pharmaceuticals (e.g., tetracyclines) with soil surfaces exemplify the potential of FTIR to characterize sorption, and thus fate, of compounds in soil.

Inorganic Molecule Interactions With Mineral Surfaces

FTIR spectroscopy has been successfully applied to inorganic ion sorption to soil surfaces, in particular the determination of sorption mechanisms (ie, inner-sphere vs. outer-sphere) of oxyanions to mineral surfaces. In cases where binding occurs and there is no change in the IR spectrum following reaction with the solid surface, outer-sphere sorption is typically taking place. The presence of new peaks or shifts in the wavenumber of existing peaks is commonly attributed to inner-sphere coordination.

The application of FTIR spectroscopy to study inorganic ion sorption to mineral surfaces is the most complete of this techniques' use in soil science, and has established the importance of pH and mineral surface charge for binding complexes of oxyanions. Oxyanions with large dipole moments (e.g., phosphate, sulfate, borate, and selenate) are particularly ideal for the FTIR study, and have been studied extensively. A salient example of insight uniquely provided by FTIR on ion sorption is the interaction of phosphate with soil minerals. FTIR studies have characterized heterogeneity in the formation of inner-sphere phosphate complexes, including the multiplicity of protonated states of such complexes and the importance of interactions with divalent metal cations (e.g., Cd^{II}).

Kinetic Studies

FTIR spectroscopy offers an approach to studying reaction kinetics of sorbates on mineral surfaces that is increasingly employed to improve on traditional batch sorption approaches. Reaction kinetics quantified by ATR-FTIR are in high agreement with those measured by conventional methods, with the added insight of molecular characterization of binding complexes. Advances in spectrometer software permit rapid collection of spectra at a time resolution that can resolve kinetics of rapid (<1 min) sorption, reduction–oxidation, and other processes that are extremely difficult to capture using conventional techniques. For example, the first application of ATR-FTIR using rapid scans (<3 s scan^{-1}) to study oxyanion sorption identified the kinetics of arsenite–arsenate oxidation on Mn oxide surfaces.

Summary

FTIR spectroscopy is a potent tool for the study of soil and soil processes. Since its initial application to study the mineral and organic components of soils in the mid-20th century, this technique offers characterization of minerals, organic matter, and processes such as mineral weathering, reduction–oxidation, and ion and organic compound binding to mineral surfaces. The high degree of experimental and analytic flexibility furnished by FTIR spectroscopy reflects the wide variety of methods for collecting spectra, and the suitability of soil components and processes to molecular analysis by infrared spectroscopy. The recent advent of ATR techniques has further advanced FTIR spectroscopy from identification and characterization of soil components and oxyanion sorption complexes to in situ, real-time analysis of soil processes occurring at liquid–solid interfaces. The molecular resolution and flexibility of experimental approaches offered by FTIR spectroscopy will likely continue to support and drive advances in soil science.

See also: AFM and Raman Spectroscopy, Applications in Cellular Imaging and Assays; ATR and Reflectance IR Spectroscopy, Applications; Chromatography-IR, Applications; Chromatography-IR, Methods and Instrumentation; Computational Methods and Chemometrics in Near Infrared Spectroscopy; Electronic Spectroscopy, Environmental Applications; Environmental and Agricultural, Applications of Atomic Spectroscopy; Far Infrared Spectroscopy Applications; Femtosecond Stimulated Raman Spectroscopy; Forensic Science, Applications of IR Spectroscopy; Forensic Science, Applications of Raman Spectroscopy to Fiber Analysis; FT-IR and Raman Spectroscopies, Polymorphism Applications; FTIR Spectroscopy of Aqueous Solutions; FT-Raman Spectroscopy, Applications; High Resolution Gas Phase IR Spectroscopy Applications; High Resolution Gas Phase IR Spectroscopy Instrumentation; High-Pressure IR; Infrared and Raman Spectroscopy of Minerals and Inorganic Materials; IR and Raman Spectroscopies, Matrix Isolation Studies; IR and Raman Spectroscopies of Inorganic, Coordination and Organometallic Compounds; IR and Raman Spectroscopies, Polymer Applications; IR and Raman Spectroscopies, Studies of Hydrogen Bonding and Other Physicochemical Interactions; IR and Raman Spectroscopies, The Study of Art Works; IR and Raman Spectroscopy, Industrial Applications; IR, Biological Applications; IR, Medical Science Applications; IR Spectral Group Frequencies of Organic Compounds; IR Spectrometers; IR Spectroscopic Data Processing; IR Spectroscopy Sample Preparation Methods; IR Spectroscopy, Surface Studies; IR Spectroscopy, Theory; Near-Infrared Spectra, Interpretation; Near-Infrared Spectroscopy; Near-IR Spectrometers; NMR of Soil Organic Matter; Nonlinear Raman Spectroscopy, Applications; Nonlinear Raman Spectroscopy, Instruments; Nonlinear Raman Spectroscopy, Theory; Protein Structure Analysis by CD, FTIR, and Raman Spectroscopies; Raman and Infrared Microspectroscopy; Raman Spectroscopy, Biochemical Applications; Raman Spectroscopy, Medical Applications: A New Look Inside Human Body With Raman Imaging; Raman Spectroscopy, Soil Analysis Applications; Spatially Offset Raman Spectroscopy; Spatially Resolved IR; Time-Resolved Raman Spectroscopy; Vibrational CD, Applications; Vibrational CD Spectrometers; Vibrational CD, Theory and Application to Determination of Absolute Configuration; Vibrational CD, Theory;

Vibrational, Rotational and Raman Spectroscopy, Historical Perspective; Vibrational Spectroscopy Applications in Drugs Analysis; Vibrational Spectroscopy, Flame and Temperature Measurement; Vibrational Spectroscopy in Food Processing.

Further Reading

Arai Y and Sparks DL (2001) *J. Colloid Interface Sci*. 241: 317–326.

Boyd SA, Johnston CT, Laird DA, Teppen BJ, and Li H (2011) Comprehensive study of organic contaminant adsorption by clays: methodologies, mechanisms, and environmental implications. In: *Biophysico-Chemical Processes of Anthropogenic Organic Compounds in Environmental Systems*, pp. 51–71. New York, NY: John Wiley & Sons Inc.

Farmer VC (1974) *The Infrared Spectra of Minerals*. London: Mineralogical Society.

Hay MB and Myneni SCB (2007) *Geochim. Cosmochim. Acta* 71: 3518–3532.

Johnston CT and Aochi YO (1996) Fourier transform infrared and Raman spectroscopy. In: Spark DL, Page AL, Helmke PA, and Loeppert RH (eds.) *Methods of Soil Analysis. Part 3 — Chemical Methods. Series 5.3*, pp. 269–321. Madison, WI: Soil Science Society of America.

Lefèvre G (2004) *Adv. Colloid Interface Sci*. 107: 109–123.

Madejová J (2003) *Vib. Spectrosc*. 31: 1–10.

Madejová J and Komadel P (2001) *Clay Clay Miner*. 49: 410–432.

McMillan, P. F. & Hofmeister, A. M. (1988). Infrared and Raman spectroscopy. In Hawthorne, F. C. (ed.) *Review in mineralogy: spectroscopic methods in mineralogy and geology*. Vol. 18, pp 99–159. Mineralogical Society of America.

Parikh, S. J., Goyne, K. W., Margenot, A. J., Mukome, F. N. D. & Calderón, F. J. (2014). Chapter One - Soil Chemical Insights Provided through Vibrational Spectroscopy. In Sparks, D.L. (ed.) *Advances in Agronomy*. Vol. 126, pp 1–148. Academic Press.

Persson P, Nilsson N, and Sjoberg S (1996) *J. Colloid Interface Sci*. 177: 263–275.

Russell JD and Fraser AR (1994) Infrared methods. In: Wilson MJ (ed.) *Clay Mineralogy: Spectroscopic and Chemical Determinative Methods*, pp. 11–67. London: Chapman & Hall.

Suarez DL, Goldberg S, and Su C (1999) Evaluation of oxyanion adsorption mechanisms on oxides using FTIR spectroscopy and electrophoretic mobility. In: Sparks DL and Grundi TJ (eds.) *Mineral-Water Interfacial Reactions*. vol. 715, pp. 136–178. Washington, DC: American Chemical Society.

Tejedor-Tejedor MI and Anderson MA (1990) *Langmuir* 6: 602–611.