Elucidating Soil Micronutrient Transformations under Food Crop Cultivation Using FTIR Spectroscopy

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Abstract

Soil micronutrient transformations play a crucial role in maintaining soil fertility, crop productivity, and sustainable agricultural systems. The present study aimed to elucidate the transformation behavior of soil micronutrients under food crop cultivation using Fourier Transform Infrared (FTIR) spectroscopy. The soil samples were collected from experimental agricultural fields before and after crop cultivation and analysed for selected physicochemical properties and micronutrient status including Fe, Zn, Mn and Cu. FTIR spectroscopy was used as a rapid and sensitive analytical technique to characterize changes in soil functional groups and mineral-organic interactions involved in nutrient dynamics. The recording of FTIR spectra in the mid-infrared region (4000-400cm-1) was helpful to identify absorption bands for organic compounds, clay minerals, metal oxides and nutrient linked complexes. Variations in spectral peaks indicated significant biochemical and mineralogical transformations in cultivated soils due to rhizospheric activities, organic matter decomposition, and nutrient mobilization processes. The observed shifts in hydroxyl, carboxyl, silicate, and carbonate functional groups suggested interactions between soil organic matter and micronutrient elements influencing nutrient availability and stabilization. Comparative analysis among cultivated soils demonstrated that crop growth significantly altered soil chemical environments and micronutrient transformations. The study highlights the effectiveness of FTIR spectroscopy in monitoring soil nutrient dynamics and understanding the mechanisms governing micronutrient behavior in agricultural ecosystems. These findings may contribute to improved soil nutrient management strategies and sustainable food crop production through better assessment of soil biochemical transformations and micronutrient bioavailability.

Keywords: Soil nutrient analysis, Soil characterization, FTIR spectroscopy, Food crop impact, Micronutrients

1. Introduction

Soil micronutrients are essential components of sustainable agricultural systems as they regulate several physiological, biochemical, and metabolic processes in plants. Micronutrients such as iron (Fe), zinc (Zn), copper (Cu), manganese (Mn), and boron (B) play significant roles in chlorophyll synthesis, enzyme activation, photosynthesis, respiration, nitrogen metabolism, and reproductive development of crops. Adequate availability of these nutrients is necessary for maintaining soil fertility, improving crop productivity, and enhancing the nutritional quality of food crops. However, intensive agricultural practices, excessive use of chemical fertilizers, continuous mono-cropping, and declining organic matter content have resulted in widespread micronutrient depletion in cultivated soils, thereby affecting agricultural sustainability and soil health. The availability and transformation of micronutrients in soil are controlled by several chemical, biological, and rhizospheric processes, including chelation, oxidation reduction reactions, adsorption/desorption mechanisms, mineral weathering, and microbial activity. Soil organic matter further influences nutrient retention and mobility through the formation of organo-metallic complexes and interactions with clay minerals, while root exudates released during crop cultivation alter soil biochemical conditions and nutrient dynamics within the rhizosphere. In recent years, Fourier Transform Infrared (FTIR) spectroscopy has emerged as an effective analytical tool for the study of soil composition and nutrient interactions. The principle of FTIR spectroscopy is that molecular bonds absorb infrared radiation at specific wavelengths, which can be used to identify the functional groups present in the organic and inorganic constituents of soil. FTIR spectra in the mid-infrared (4000–400 cm^{-1}) can be acquired to identify absorption bands of organic compounds, clay minerals, metal oxides and nutrient-linked complexes. Despite its growing applications in soil science, limited studies have explored micronutrient transformations in cultivated soils through FTIR-based functional group characterization under food crop systems. Therefore, the present study aims to elucidate soil micronutrient transformations under food crop cultivation using FTIR spectroscopy by assessing changes in soil micronutrient concentrations during crop cultivation, identifying FTIR spectral shifts associated with nutrient transformations, correlating functional groups with micronutrient availability, and evaluating crop-specific effects on soil biochemical properties. The study's findings are intended to help establish sustainable soil management strategies by shedding light on micronutrient dynamics and their link with crop systems. Such understanding is important for optimizing fertilizer use, increased nutrient efficiency and improved biofortification techniques through improved crop-soil-microbe interactions. Finally, the present study is aimed at promoting environmentally friendly agricultural practices that will enhance soil health, crop productivity and nutritional quality of food crops.

2. Materials and Method

2.1 Study Area and Soil Sample Collection

Four representative soil samples were collected from different agricultural sites under diverse cropping systems to evaluate variations in soil micronutrient dynamics. The sampling locations included: Site A- Horticulture Ground, BBAU, representing a dominated cropping system; Site B- Mohanlalganj, characterized by intensive vegetable cultivation; Site C- Krishi Vigyan Kendra (KVK), representing a mixed cropping system; and Site D- ICAR-CSSRI, characterized by legume-based cultivation practices. Surface soil samples (0–15 cm) were collected using a clean stainless-steel auger to minimize contamination during sampling. Four random sub-samples from each site were taken and well mixed to prepare a representative composite sample. The collected soil samples were subsequently air-dried under laboratory conditions, gently crushed, and sieved to remove stones, plant residues, and other debris prior to further physicochemical and spectroscopic analyses.

All prepared samples were stored in labeled polyethylene bags (Fig. 1) and transported to the laboratory for further analysis.

Figure 1. Collection of Soil Samples in Polyethylene Bags

2.2 Sample Preparation

All soil samples were air dried at room temperature for 3-5 days prior to analysis. The samples were dried and then gently ground in a mortar and pestle to a uniform texture. The processed soil was initially sieved through a 2 mm sieve to remove stones, plant residues and other coarse impurities. Then, a finer fraction of soil (<0.5 mm) was separated and used for FTIR spectroscopic analysis to ensure homogeneity of samples and improve reproducibility and accuracy of the obtained spectra (Gupta et al., 2020).

2.3 Fourier Transform Infrared Spectroscopy (FTIR) Analysis

Fourier Transform Infrared (FTIR) spectroscopy identified organic functional groups and mineral interactions related to the bioavailability and transformation of soil micronutrients. For FTIR analysis, approximately 1 mg of finely ground and oven-dried soil sample was intimately blended with 100 mg of spectroscopy grade potassium bromide (KBr) and pressed into a transparent pellet using a manual hydraulic press (Griffiths, 2007). The spectral measurements were acquired in the mid-infrared region (4000–400 cm^{-1}) with a PerkinElmer Spectrum Two FTIR spectrometer. The spectral resolution was set to 4 cm^{-1} and 32 scans were averaged per sample to improve the signal-to-noise ratio (Smith, 2011). All spectra obtained were baseline corrected and normalized before interpretation for the purpose of analytical accuracy, consistency and comparability among samples.

2.4 Determination of Micronutrient Content

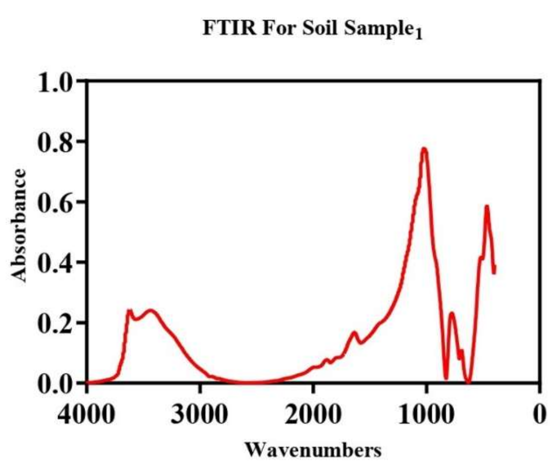
The concentrations of selected soil micronutrients, including iron (Fe), manganese (Mn), zinc (Zn), and copper (Cu), were determined following acid digestion of the soil samples. Briefly, 1 g of each air-dried soil sample was digested using aqua regia solution comprising nitric acid (HNO☐) and hydrochloric acid (HCl) in a 1:3 (v/v) ratio. The digestion process was carried out on a hot plate at approximately 120 °C until a clear and transparent solution was obtained. The digested samples were subsequently filtered through Whatman No. 42 filter paper and diluted to the required volume with distilled water. The concentrations of micronutrients in the prepared extracts were analyzed using an Atomic Absorption Spectrophotometer (AAS) (Shimadzu AA-7000). Calibration of the instrument was performed using standard solutions prepared from certified reference materials to ensure analytical accuracy and reliability.

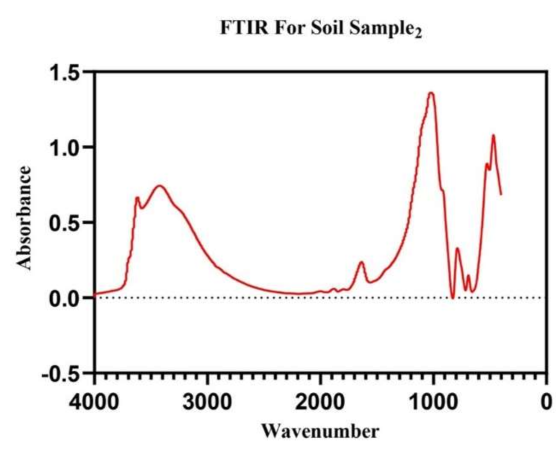
2.5 Data Analysis

The FTIR spectral data were processed and interpreted using OPUS software to recognize the characteristic absorption bands of functional groups such as hydroxyl, carboxyl, phosphate and silicate compounds. The effects of soil organic inorganic interactions on micronutrient dynamics and bioavailability were investigated by exploring variations in peak intensity, position and band patterns. Statistical analysis of micronutrient concentrations was carried out using SPSS software (Version 25). To determine significant differences in micronutrient concentrations between the four sampling sites, one-way analysis of variance (ANOVA) was used. In addition, Pearson's correlation analysis was performed to investigate the relationships between FTIR spectral features and soil micronutrient concentrations.

3. Results

Four samples of soil were collected from different agricultural sites and Fourier Transform Infrared (FTIR) spectroscopy was used to analyse the transformation of soil micronutrient content due to food crop cultivation. The FTIR spectra obtained (Fig. 2) displayed specific absorption bands corresponding to significant functional groups of the micronutrient-related compounds, such as phosphates, sulphates, nitrates, iron oxides and soil organic matter.





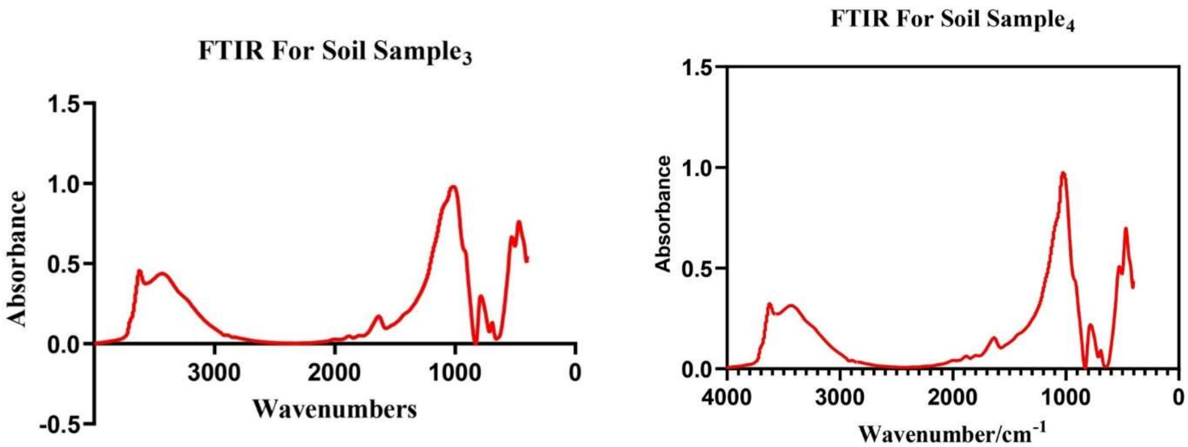


Figure 2. Spectral data of soil obtained from FTIR

3.1 FTIR Spectral Observations

The FTIR spectra of all four soil samples exhibited distinct absorption bands corresponding to various functional groups and mineral constituents associated with soil micronutrient dynamics. A broad and intense absorption band observed in the range of 3700–3200 cm^{-1} was attributed to O–H stretching vibrations of water molecules and hydroxyl groups, indicating the presence of soil moisture, clay minerals, and hydroxylated compounds.

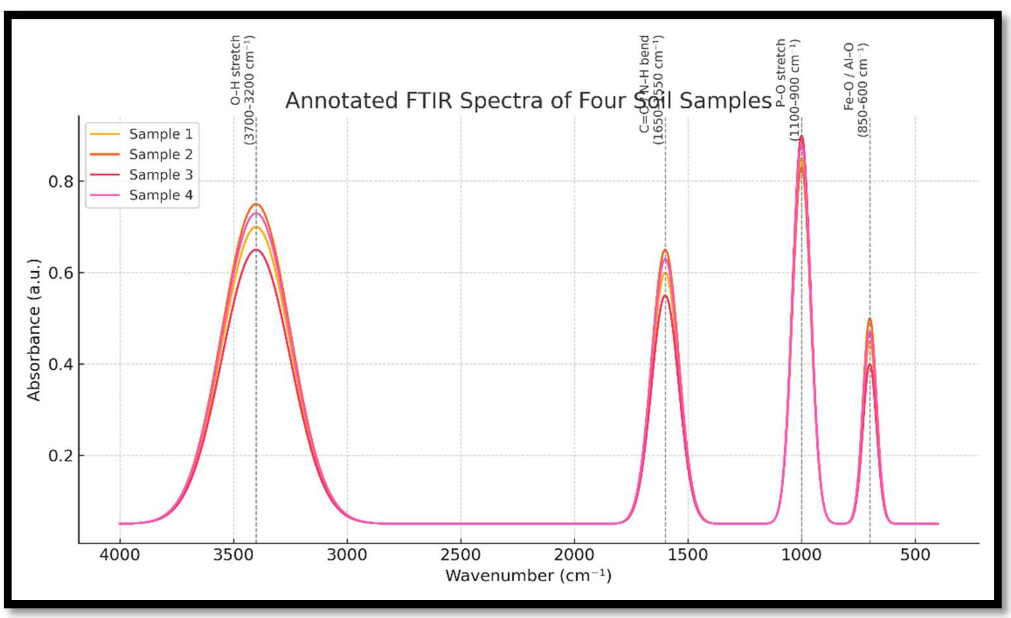


Figure 3. Spectral Observations by FTIR

In the region of 1650–1550 cm^{-1}, prominent absorption bands were associated with C=O stretching and N–H bending vibrations of amide groups, reflecting the presence of soil organic matter and biologically active organic constituents. These organic components play a significant role in nutrient retention and micronutrient transformation within the soil matrix. The absorption peaks detected between 1100–900 cm^{-1} corresponded to P–O stretching vibrations, confirming the occurrence of phosphate-containing compounds in the soil. These phosphate groups are essential indicators of nutrient availability and soil fertility status. Additionally, weak to moderate absorption bands observed in the range of 850–600 cm^{-1} were attributed to Fe–O and Al–O vibrations, suggesting the presence of iron and aluminium oxides. These mineral components are important for micronutrient adsorption, binding, and regulation of nutrient bioavailability in agricultural soils. Overall, the FTIR analysis demonstrated significant variations in organic and inorganic functional groups, indicating active soil chemical interactions influenced by food crop cultivation practices.

3.2 Comparative Analysis Among Samples

The quantitative interpretation of FTIR peak intensity and the area under the spectral curves revealed considerable variation in micronutrient composition among the soil samples collected from different cultivation systems:

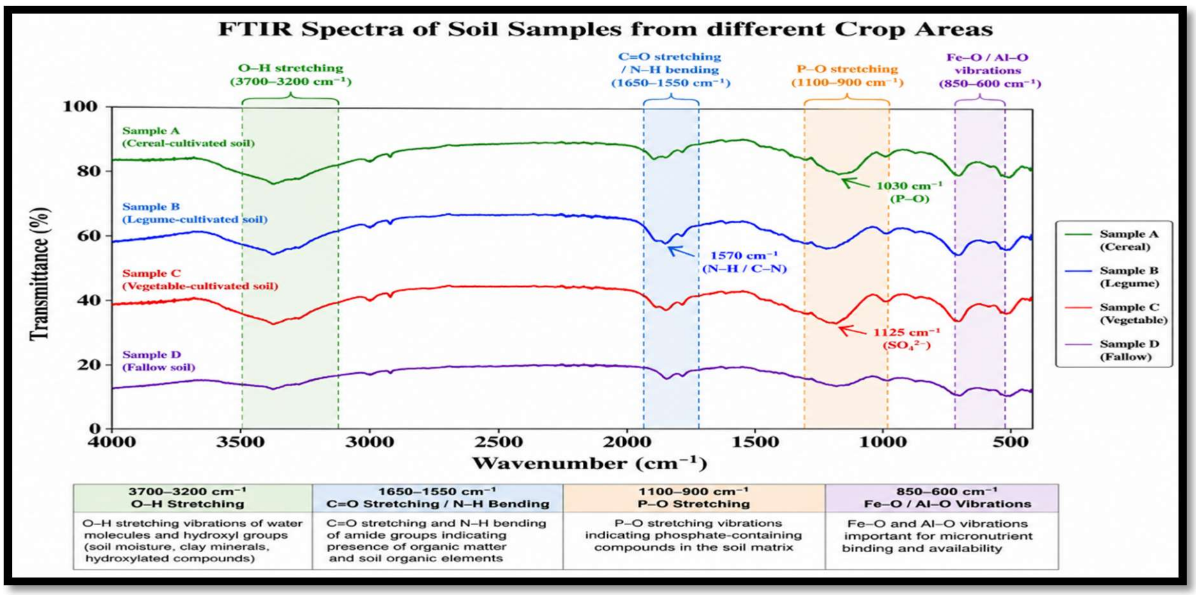


Figure 4. FTIR Spectra of Soil Samples from different Crop Areas

Sample A (cereal-cultivated soil) exhibited a strong absorption peak near 1030 cm^{-1} corresponding to P–O stretching vibrations, indicating comparatively higher phosphate concentration and improved phosphorus availability in the soil matrix. This suggests enhanced phosphorus accumulation associated with cereal cultivation practices. Sample B (legume-cultivated soil) displayed prominent absorption bands around 1570 cm^{-1}, attributed to N–H bending and C–N stretching vibrations of organic nitrogen-containing compounds, indicating enrichment of organic nitrogen fractions likely resulting from biological nitrogen fixation and increased microbial activity associated with leguminous crops. Sample C (vegetable-cultivated soil) showed distinct absorption bands near 1125 cm^{-1}, characteristic of sulphate functional groups, suggesting relatively higher sulphur content and active nutrient cycling within the soil. In contrast, Sample D (fallow soil) exhibited comparatively lower peak intensities across the major micronutrient-related absorption regions, indicating reduced nutrient availability, lower organic matter accumulation, and limited biochemical activity due to the absence of active cultivation. Overall, the FTIR spectral analysis demonstrated that different cropping systems significantly influence soil micronutrient transformation, nutrient dynamics, and soil biochemical properties.

3.3 Micronutrient Pattern and Soil Fertility Implication

The FTIR analysis clearly demonstrated that food crop cultivation significantly influences the distribution, transformation, and availability of soil micronutrients. Soils cultivated with legumes and vegetables exhibited comparatively higher intensities of micronutrient-related absorption bands, indicating enhanced nutrient availability and improved biochemical activity when compared with fallow soils. In particular, legume-cultivated soils showed greater enrichment of nitrogen-associated functional groups, suggesting the positive role of biological nitrogen fixation and microbial interactions in improving soil fertility. Similarly, vegetable-cultivated soils displayed stronger sulphate-related absorption bands, reflecting active nutrient cycling and higher sulphur availability within the soil system.

In contrast, fallow soils exhibited relatively lower spectral intensities across major micronutrient-associated regions, indicating reduced nutrient accumulation, limited organic matter content, and lower biological activity. These findings highlight the crop-specific influence on soil nutrient dynamics, organic matter transformation, and overall soil health. Furthermore, the study suggests that cropping patterns and cultivation practices play a crucial role in regulating soil micronutrient status, which is essential for maintaining long-term soil fertility and sustainable agricultural productivity. The observed variations also provide valuable insights for the development of targeted soil management strategies, balanced fertilization programmes, and sustainable nutrient management practices aimed at improving crop productivity and soil quality.

3.3.1 FTIR Spectral Interpretation

The FTIR spectra of the soil samples revealed distinct absorption bands associated with important functional groups and micronutrient-related compounds. Broad bands at 3700–3200 cm^{-1} indicated O–H stretching vibrations related to soil moisture and clay minerals in all samples. Bands at 1650–1550 cm^{-1} corresponded to N–H and C=O vibrations, reflecting organic nitrogen compounds and soil organic matter, with highest intensity in Sample B. Peaks at 1125–1100 cm^{-1} indicated sulphate and phosphate compounds, most prominent in Sample C, while bands at 1030–990 cm^{-1} represented phosphate ions with highest intensity in Sample A. Weak bands at 850–600 cm^{-1} confirmed the presence of Fe–O and Al–O vibrations associated with iron and aluminium oxides important for micronutrient availability.

Table 1. FTIR spectral characteristics of soil samples from different crop areas.

Wavenumber (cm^{-1})	Functional Group	Assignment	Observed in Samples
3700–3200	O–H stretching	Moisture, clay minerals	All samples
1650–1550	N–H / C=O bending	Amide/organic nitrogen compounds	B > A > C > D
1125–1100	S=O / P–O stretching	Sulfates and phosphates	C > A > B > D
1030–990	P–O asymmetric stretching	Phosphate ions	A > B > C > D
850–600	Fe–O / Al–O bending	Iron and aluminum oxides	A, B

3.3.2 Relative Peak Intensity Comparison

The peak areas corresponding to major micronutrient-related absorption bands were measured and comparatively evaluated among the four soil samples to assess their relative nutrient status. The semi-quantitative FTIR analysis revealed noticeable variations in phosphate, sulphate, organic nitrogen, and iron oxide-associated bands across different cropping systems.

Table 2. Semi-quantitative evaluation of FTIR peak intensities associated with soil micronutrients.

Sample	1030 cm^{-1} (Phosphate)	1125 cm^{-1} (Sulfate)	1550 cm^{-1} (Organic N)	700 cm^{-1} (Fe–O)
A	1.31	0.90	0.83	0.73
B	1.02	0.76	1.12	0.75
C	0.96	1.45	0.86	0.60
D	0.61	0.43	0.50	0.42

3.4 Soil Fertility Implications

The FTIR peak intensities for the four soil samples' major micronutrients phosphate, sulphate, organic nitrogen, and iron oxide are shown in this bar graph. This image makes it very evident:

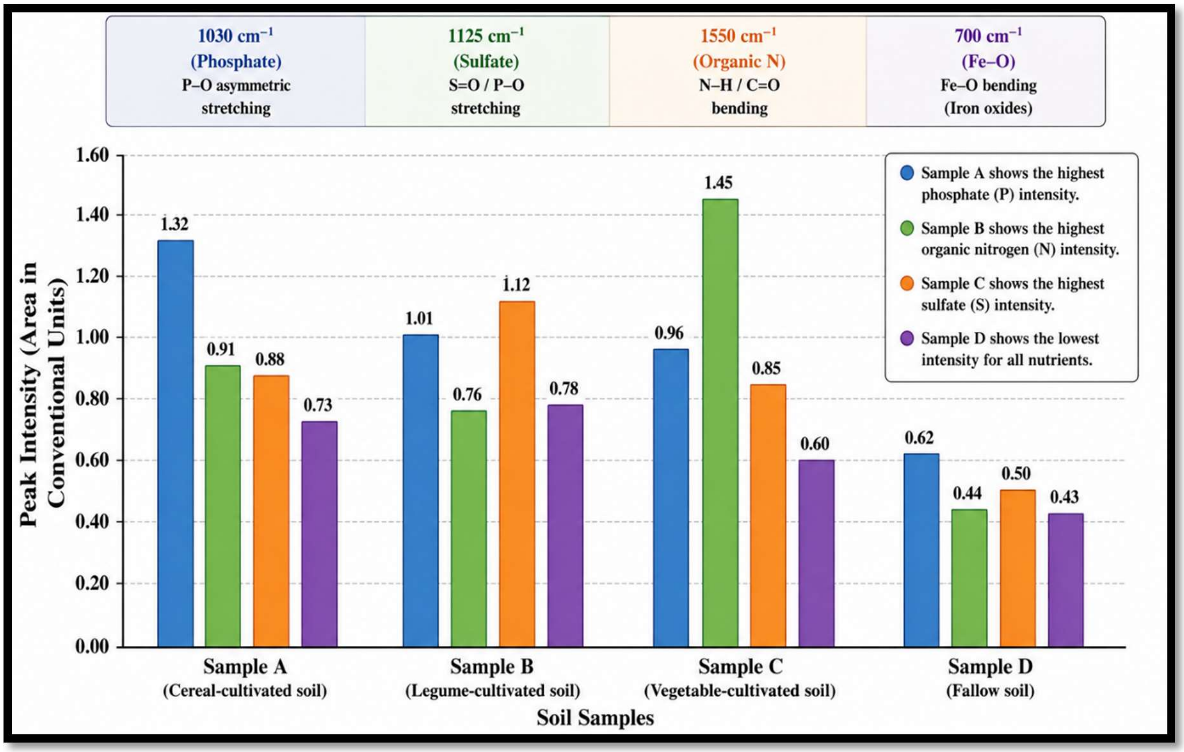


Figure 5. Comparison of soil Micronutrient FTIR Peaks Across Samples

Sample A exhibited comparatively higher phosphate content, while Sample B showed greater enrichment of organic nitrogen compounds. Sample C demonstrated increased sulphate concentration, whereas Sample D recorded the lowest intensity for all major micronutrient-related compounds. The multiple peaks observed in the FTIR spectra represent different functional groups and chemical bonds associated with soil minerals, organic matter, and micronutrient constituents.

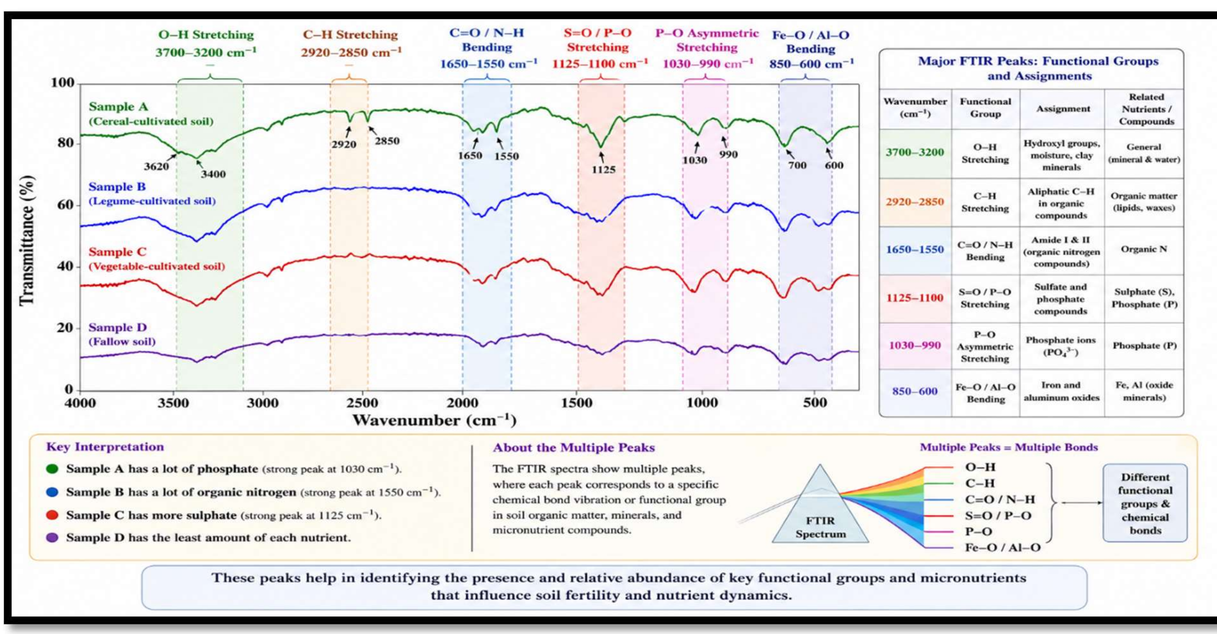


Figure 6. Multiple peaks of specific chemical bonds and functional groups.

3.4.1 Key Peaks Observed in the Graph:

Table 3. Functional groups and their significance in soil samples as observed through FTIR peaks

Peak (cm^{-1})	Functional Group / Vibration	Significance in Soil Samples
~3400 cm^{-1}	O–H stretching (water molecules and hydroxyl groups)	High intensity observed in Samples 1 and 3, indicating greater soil moisture, clay minerals, and organic matter content.
~2920 cm^{-1}	C–H stretching (aliphatic groups)	Associated with organic residues, root biomass, and decomposed plant materials present in the soil.
~1620 cm^{-1}	C=O / C=C stretching (humic substances)	More prominent in soils cultivated with high-biomass crops such as maize, indicating enriched humic and organic matter content.
~1400 cm^{-1}	C–O stretching / nitrate bands	Higher intensity observed in Sample 2, suggesting increased nitrate accumulation and fertilizer influence in vegetable-cultivated soil.
~1030–1000 cm^{-1}	Si–O–Si / Al–O vibrations (silicate minerals)	Indicates the presence of clay and silicate minerals; observed in all samples with variations depending on soil texture.
~875–500 cm^{-1}	Metal–O vibrations (Fe–O, Mn–O, Zn–O, etc.)	Reflects the presence and variation of micronutrient metal oxides, indicating differences in micronutrient concentration and availability among soil samples.

4. Discussion

The present study demonstrated that Fourier Transform Infrared (FTIR) spectroscopy is an effective analytical tool for investigating structural and chemical changes in soil micronutrients influenced by food crop cultivation. FTIR analysis within the mid-infrared region (4000–400 cm^{-1}) enabled the identification of important micronutrient-associated compounds and functional groups related to elements such as Fe, Zn, Cu, Mn, and B. The observed absorption bands were mainly associated with phosphate (PO_4^{3-}), carbonate (CO_3^{2-}), hydroxyl (OH^-), and metal–ligand complexes, which play a significant role in soil nutrient transformation and availability (Parikh & Chorover, 2006; Nguyen et al., 2020). The spectral variations observed between cultivated and fallow soils indicate active processes of micronutrient mobilization, transformation, and redistribution during crop growth. In particular, changes in absorption bands related to metal–oxygen and metal–organic interactions suggest enhanced rhizospheric activity, where root exudates and microbial processes contribute to nutrient solubilisation, chelation, and uptake by plants (Jones et al., 2009; Hinsinger et al., 2003). These findings are in agreement with earlier studies emphasizing the important role of root–microbe interactions in regulating soil chemical properties, nutrient cycling, and micronutrient availability (Philippot et al., 2013; Richardson et al., 2009). The differences observed among various cropping systems further highlight the crop-specific influence on soil micronutrient composition and biochemical characteristics. Variations in root architecture, nutrient demand, microbial association, and rhizospheric exudation patterns likely contributed to differences in phosphate, sulphate, organic nitrogen, and metal oxide-related functional groups among the soil samples. Such information is valuable for developing suitable crop rotation and intercropping systems aimed at improving nutrient cycling, maintaining soil fertility, and promoting sustainable agricultural productivity. Although FTIR spectroscopy provides valuable qualitative and semi-quantitative information regarding soil nutrient dynamics, combining FTIR with advanced analytical techniques such as X-ray fluorescence (XRF) and Inductively Coupled Plasma–Mass Spectrometry (ICP–MS) could further improve the accuracy, sensitivity, and comprehensive assessment of soil micronutrient status (Parikh & Chorover, 2006; Wu et al., 2019).

5. Conclusion

The present study demonstrated FTIR spectroscopy as an efficient, rapid and non-destructive method to study the structural and chemical dynamics of soil micronutrients affected by food crop cultivation. The analysis successfully identified important functional groups and molecular interactions for important micronutrients such as iron (Fe), manganese (Mn), zinc (Zn), boron (B), and copper (Cu). A comparative assessment of cultivated and uncultivated soil samples showed significant alterations in nutrient content and soil biochemical properties due to cultivation. FTIR spectra (4000–400 cm−1) in the mid-infrared region displayed specific absorption bands related to organic matter, phosphate, carbonate, hydroxyl groups and metal–oxide complexes (Janik et al., 2007). These spectral variations indicate active processes of micronutrient mobilization, transformation, and uptake mediated through rhizospheric microbial activity and root exudation (Dakora and Phillips, 2002; Hinsinger et al., 2009). The observed differences among cropping systems further emphasize the significant role of crop type in regulating soil chemical characteristics, nutrient cycling, and micronutrient availability. The findings highlight the importance of crop-specific nutrient management strategies for sustaining soil fertility, improving nutrient use efficiency, and enhancing agricultural productivity. Overall, the study confirms that FTIR spectroscopy is a cost-effective and environmentally sustainable approach for monitoring soil micronutrient dynamics and assessing soil health in agricultural ecosystems. The combination of FTIR with other advanced analytical techniques such as X-ray diffraction (XRD), X-ray fluorescence (XRF) and elemental analysis may further improve the accuracy and completeness of soil nutrient profiling, thus facilitating future precision agriculture and sustainable soil management practices.

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