



# From Soil to Spectrum: Decoding the Impact of Nutrient Management Practices and Herbicides using FTIR

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## ABSTRACT

**Background:** FTIR spectroscopy is the instrumental technique used in science for studying soil constituents and their variations rapidly. Being a non-extraction technique, FTIR could also be used to study the interaction of soil composition with the applied external inputs like fertilizer nutrients through organic and inorganic sources and herbicides by assessing the variations in spectral patterns. This will also reveal the type of interaction and changes taking place in soil swiftly. Hence, the current study was carried out to investigate the interaction of herbicides with soil components under various fertilizer nutrient management practices.

**Methods:** Three herbicides (glyphosate, pendimethalin, metribuzin) were applied to the sandy loam soil treated with soil inorganic fertilizer (NPK+MN) and organic fertilizer (NPK+FYM). Treated soils along with control, were collected, processed and subjected to FTIR analysis. Based on the intensity of absorption changes, the type of interactions and changes that occurred in the soil were assessed.

**Result:** Results of the study reveal that the application of herbicides (glyphosate, pendimethalin and metribuzin) to soil and NPK + micronutrients and NPK + FYM resulted in complex interactions and changes in FTIR absorption intensities, notably in fingerprint regions (1200-400 cm<sup>-1</sup>). Shift in the peaks at different wave numbers occurred due to the interaction of soil constituents with the herbicides and organic matter as FYM. The study highlights that a deeper understanding of these complex interactions is crucial for optimizing the use and time of application of fertilizer nutrients and herbicides, minimising environmental impacts and promoting sustainable agricultural practices that preserve soil health and productivity.

**Key words:** Fertilization, FTIR, FYM, Herbicides, Nutrients, Soil.

## INTRODUCTION

The extensive use of herbicides in modern agriculture has considerably contributed to weed control, crop yield enhancement and food security. Herbicides such as glyphosate, pendimethalin and metribuzin are widely used because they are effective against a wide range of weeds and grasses. However, their use can cause soil pollution and harm soil health and microbial activity. Furthermore, improper herbicide use and a lack of rapid herbicide residue and persistence analysis could further exacerbate environmental concerns. Application of two more herbicides in sequence and or combination as tank mixes has been a standard practice for improving weed control performance while lowering the danger of herbicide resistance. Besides, the farmers are also adopting different nutrient management practices, viz., soil test-based nutrient sources with and without organic manures, which will have a varied effect on herbicide dynamics and behavior in soil.

The soil components such as clay minerals, organic matter, metallic oxides and humic substances are the sites and sources on which herbicides are adsorbed or absorbed typically after application. The water-solubility, metal complexation and adsorption qualities are crucial in regulating the rate of transport process in soil (Barja and Santos Afonso, 1998). Chromatographic analyses of herbicide residues will give information only on the persistence and residues in soil but not the changes that

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occur in soil due to their interaction with chemical properties. Fourier Transform Infrared (FTIR) spectroscopy has recently come into prominence as a viable non-extraction technique for studying the herbicide interaction with soil components (Cannane *et al.*, 2013) and management practices (Raphael,

2011). Also, the FTIR technology could be optimized for non-destructive detection of herbicide residues in soil based on changes in patterns of spectra.

The significant adsorption of glyphosate (GPS), a commonly used herbicide, to soil components, where microorganisms swiftly degrade it, is thought to be the cause of its low phytotoxicity in soils (Carlisle and Trevors, 1988). It is believed that the phosphonate group is responsible for adsorption in sediments and soils, which would account for the competition between inorganic phosphate and GPS adsorption sites (Sprankle *et al.*, 1975; Torstensson, 1985). Furthermore, the presence of amino, carboxylic and phosphonic compounds in its structure can form strong complexes with transition metals, which can coordinate singly with metal ions or in combination as a bidentate or tridentate ligand (Madsen *et al.*, 1978; Motekaitis and Martell, 1985). The IR spectrum study on glyphosate-copper complexes reveals the involvement of the GPS molecule in carboxylate and phosphonic moieties. The complex formation results in a decreased symmetry in the phosphonate group due to the loss of the resonance situation of  $\text{PO}_3^{2-}$  groups, resulting in a split of their absorption bands. Pendimethalin (PM) is a dinitroaniline herbicide, commonly used for the pre-emergence control of seedling grass and broad-leaved weeds in several broad-leaved crops and in corn, sugar cane and spring wheat. Pendimethalin is strongly adsorbed by most soils and its sorption is correlated to organic matter and clay content. Studies have reported that soil organic carbon content can significantly affect the sorption and mobility of pendimethalin. Rytwo *et al.* (2005) studied the adsorption of pendimethalin on montmorillonite through FTIR measurements and revealed that its interactions are via the nitro and methyl groups. Metribuzin is a selective herbicide commonly used in various crops to control broadleaf weeds. Its adsorption in the soil is influenced by factors such as soil pH, organic matter content and clay mineralogy. High organic matter content can enhance the retention of metribuzin, reducing its bioavailability for weed control. On the other hand, soil pH can affect its dissociation, leading to changes in its sorption behaviour.

With this background, the present study was carried out to find gaps in knowledge regarding the complex interactions between herbicides and soil components, especially in the context of varying nutrient management practices through FTIR analysis. It aims to provide valuable insights about the herbicide use while considering soil health and environmental sustainability in agriculture.

## MATERIALS AND METHODS

### Experiment details

The soil samples were collected from the experimental field before tomato transplanting and processed using a 2 mm sieve to remove the debris and heterogeneity. In the laboratory study, we utilized a uniform and processed soil

sample weighing 5 kg per pot and tomato hybrid Darsh Gold as a test crop under a controlled transparent glass house at Dept of Soil Science and Agricultural Chemistry, TNAU, Coimbatore by imposing the treatments *viz.*, two nutrient management practices with and without herbicides spray along with absolute control. The nutrient management practices imposed were i). NPK (nitrogen, phosphorus and potassium) fertilizers @ 203, 238 and 150 kg/ha respectively and micronutrients (MN) fertilizers *viz.*,  $\text{ZnSO}_4$  50 kg/ha, Borax 10 kg/ha,  $\text{CuSO}_4$  3.75 kg/ha and ii). NPK fertilizers + Farm Yard manure (FYM) @ 25 t/ha. Fertilizer nutrients were applied on the day of tomato transplanting, while FYM was applied ten days before the transplanting of tomato. The herbicide *viz.*, glyphosate was applied one week before transplanting as a pre-plant herbicide and pendimethalin and metribuzin were applied as pre-emergence on 3<sup>rd</sup> day after tomato transplanting. The NPK nutrients were applied through urea, single super phosphate and muriate of potash respectively. The commercial formulations of herbicides *viz.*, glyphosate 41% SL, pendimethalin 50% EC and metribuzin 70% WP were used for the study and were sprayed on the soil surface with a spray volume of 500 L/ha. On 3<sup>rd</sup> day after imposing all the treatments, the soil sample was collected from each pot up to 15 cm depth and processed to a fine powder after air drying using a pestle and mortar for FTIR analysis. The experiment was conducted over the course of one growing season.

### Soil characteristics

The processed soil was also sub-sampled and analyzed for the initial physicochemical characteristics. The soil is classified as *alfisol* and has a sandy loam texture, medium available N (263 kg/ha) and high available P (30 kg/ha) and K (420 kg/ha) status. It was also observed to be non-saline (EC 0.22 dS/m) in nature and alkaline in reaction (pH 7.55) and has CEC of 15.0cmol/kg soil.

### FTIR measurements and processing of data

The Jasco FT/IR - 6800 was used to analyze the samples and data was acquired using Spectra Manager II software. The detector used for the analysis is TGS (Triglycine sulfate). All spectra were captured over the 4000 - 400  $\text{cm}^{-1}$  ranges with a spectral resolution of 4  $\text{cm}^{-1}$  and the 1024 scans. Finely powdered soil was fed directly into the iR window of FTIR. The spectral data obtained from the instrument software and PCA analysis was processed by Origin Pro (2023) software for extracting spectra and comparison. Additionally, the Spectrograph 1.2.16.1 version was used for comparing spectra by overlapping and subtraction techniques.

## RESULTS AND DISCUSSION

### Spectral characteristics of experimental soil

The experimental field soil (control) was collected, before imposing the nutrient management practices and herbicides, processed and analyzed in FTIR to know its composition and corresponding functional groups (Fig 1). The major

absorption peaks/bands observed in the blank soil were compared and assigned with corresponding functional groups based on prior published literature (Table 1). The dominant minerals present in the experimental soil are silicates and carbonates, besides having a considerable amount of Fe-containing minerals. The absorption peaks at 524-533, 692, 781, 998, 1643, 3613-3620 $\text{cm}^{-1}$  wave numbers were commonly observed in the control soil.

The interval between the 450 and 550  $\text{cm}^{-1}$  absorption bands could be attributed to angular deformation or combinations of Si-O bonds with metal ions like Al, Fe and Mg. In the present study, the absorption band at 527 and 431  $\text{cm}^{-1}$  might represent the Al-O-Si / Fe-O-Si/Si-O-Si vibrations associated with the stretching of the oxygen bonds within the soil crystal lattice; (Schwertmann and Taylor, 1989; Schwetmann and Cornell, 1991). Peternella, (2021) reported

that the bands at 530 and 434  $\text{cm}^{-1}$  are due to the deformation of the Al-O-Si and Si-O-Si bonds, respectively. The strong stretching vibration at 1005  $\text{cm}^{-1}$  and a small peak at 1632  $\text{cm}^{-1}$  could be assigned to the silicate clays like quartz, feldspars, etc (Cannane *et al.*, 2013) and deformation of the OH group, respectively. Normally the stretching vibrations occur due to the presence of a combination of minerals. Hence, it is difficult to diagnose specific minerals, but the pattern is specific to soil type and is used to assess the management influence. The weak deformation at 775 and 692  $\text{cm}^{-1}$  could be due to the quartz mineral and indicates the existence of Si-O-Si bending vibrations. The weak stretching vibrations due to structural OH groups between 3783-3614  $\text{cm}^{-1}$  indicate the presence of clay minerals (aluminosilicates) like illite or kaolinite in the soil. Similar results of 3630, 1890, 800, 1370 and 695  $\text{cm}^{-1}$  for clay, silica,

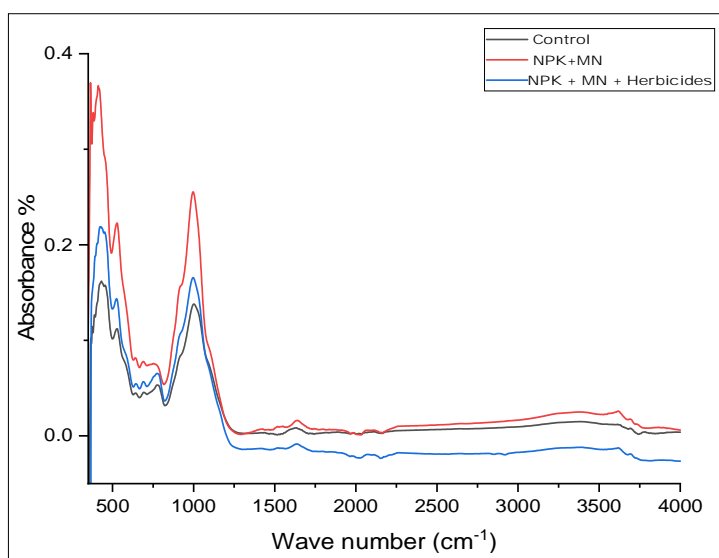


Fig 1: Comparison of FTIR Spectra of soil treated with herbicides and nutrient management practices.

Table 1: Comparison of the spectra of the observed soil samples with mid-infrared absorption assignments based on prior literature.

Observed wave number ( $\text{cm}^{-1}$ )	Components	References
3616	structural stretching of hydroxyl groups (OH)	Peternella, (2021)
3398	stretch (OH) of water	Peternella, (2021)
1643	amide, aromatic -C=C- stretching	Du <i>et al.</i> (2014); Krivoshein <i>et al.</i> (2020)
1515	amide II, aromatic rings, carboxyl C	Krivoshein <i>et al.</i> (2020)
998	C-H bending (out-of-plane)	
779 - 781	C-H out-of-plane bending vibration in an aromatic ring.	Semmler <i>et al.</i> (1991)
727	C-H bending (aromatic)	Krivoshein <i>et al.</i> (2020)
642	$\text{SiO}_2$ (Si-O) bending, iron oxide	Saikia and Parthasarathy (2010)
572	Carbon-sulfur (C-S) bond stretch	Nandiyanto <i>et al.</i> (2019)
524, 525	Fe-O vibrations / AlOSi deformation/ SiOSi deformation	Schwertmann and Cornell, (1991); Schwertmann and Taylor (1989)
		Peternella, (2021)
430	Angular deformation or combinations of Si-OM bonds, where (M = Al, Fe and Mg)	Peternella, (2021)

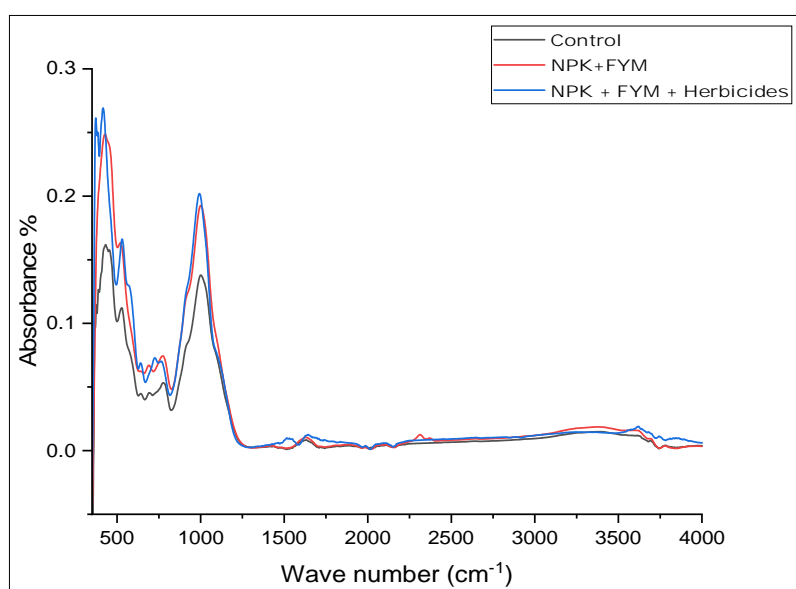
phenolic/carboxylate and silica bands were reported in clay soil by Parikh *et al.* (2014). Nuzzo *et al.* (2020) also attribute the bands below  $900\text{ cm}^{-1}$  ( $800, 780, 695, 470$  and  $430\text{ cm}^{-1}$ ) in soil to quartz and silicates.

### Influence of nutrient management practices and herbicides on soil spectral characteristics

When the herbicides are applied together, they can interact with various soil components and compete for adsorption sites on soil particles or organic matter. Each herbicide has its specific chemical properties, including molecular structure, charge and hydrophobicity, which influence its affinity for soil surfaces. The three herbicides may have different adsorption capacities and preferences for specific soil components. As a result, they may compete for available binding sites, leading to differences in absorption intensity at various wave numbers. Hence, the soil treated with

different nutrient management practices and herbicides was subjected to FTIR analysis to understand their interaction with soil components and changes in soil functional groups. Also, the observed absorption peaks might provide valuable insights into the changes in the soil's chemical composition and the interactions between the applied treatments and the soil matrix.

FTIR analysis of the soil treated with NPK + micronutrients and NPK + FYM were applied with three herbicides *viz.*, glyphosate, pendimethalin and metribuzin, yielded several absorption peaks at specific wave numbers (Fig 2). This indicates the changes in the pattern of vibrations by the distinct functional groups and chemical bonds occurring due to their applications. Soil treated with nutrients, manures and herbicides produced additional peaks at  $642, 1535, 2114$  and  $2314\text{ cm}^{-1}$  (Table 2) over blank soil but with varying absorption intensity.



**Fig 2:** Comparison of FTIR spectra of soil treated with herbicides and nutrient management practices.

**Table 2:** Intensity of absorbance peaks in soil using FTIR spectroscopy after herbicide application.

Observed wave number ( $\text{cm}^{-1}$ )	Observed Intensity				
	Control	NPK + MN	NPK + MN+ Herbicides	NPK + FYM	NPK + FYM + Herbicides
524-533	0.11	0.21	0.13	0.16	0.14
572	-	-	-	0.01	0.12
642	0.04	0.08	0.05	-	0.05
690	-	0.04	-	0.03	-
727	-	-	-	-	0.07
781-785	0.05	-	0.06	0.07	0.06
998-1005	0.13	0.25	0.16	0.19	0.20
1515	-	-	-	-	0.09
1643	0.007	0.015	-0.008	0.015	0.001
2317	-	-	-	0.012	-
3613	-	-	-	-	0.018
3625	-	0.02	-0.01	-	-

When soil is treated with NPK+MN and NPK+MN+ herbicides, the intensity of absorption at both fingerprint and grouping regions was found to be higher in NPK+MN-treated soil than in NPK+MN+ herbicides and control soils. However, no change in the pattern of absorption spectra was noticed among the above treatments, which showed that the added nutrients fertilizer didn't contribute to the change in soil functional groups. The lower intensity of peaks at all the absorbed bands in NPK+MN+ herbicides treated soil over control and NPK+MN could be attributed to the interaction of herbicides with micronutrient cations and soil components through complexation/chelation and or adsorption etc. The NPK+MN, NPK+FYM, NPK+MN+ herbicides and NPK+FYM+ herbicides treated soils showed higher intensity of absorption at 418, 530, 995, 1643 and 3616  $\text{cm}^{-1}$  over blank soil. Among the nutrient practices and herbicide treatment, the intensities were usually found to be higher with the nutrient management practices *viz.*, NPK+MN and NPK+FYM. Upon inclusion of herbicides into these nutrient management practices, a slight decrease in absorption intensity was observed except at 1643  $\text{cm}^{-1}$ . Similarly, the NPK+FYM+ herbicides displayed an additional sharp, small absorption peak at 2313  $\text{cm}^{-1}$ .

The increased intensity of absorption peaks at 411 and 530  $\text{cm}^{-1}$  indicated the interaction of added Fe with the Si-O-Si bonds within the crystal lattice of minerals in the soil. When herbicides, such as glyphosate, pendimethalin and metribuzin, are applied, they might interact with these iron minerals through adsorption, complexation and redox reactions and the same is revealed by the increased intensity of absorption. These interactions can influence herbicide mobility, stability and availability in the soil, thereby affecting their effectiveness in weed control and potential environmental risks. The slight deformation observed at 572  $\text{cm}^{-1}$  in NPK+FYM could be due to the presence of the carbon-sulfur (C-S) bond (Nandiyanto *et al.*, 2019), assigned to the  $\text{SO}_4$  addition through FYM. Also, the NPK+FYM+herbicides treated soil had increased intensity than NPK+FYM alone and might indicate the interaction of the S atom within the chemical structure of herbicide, specifically within the triazine ring of metribuzin to the soil components. The observed peak at 642  $\text{cm}^{-1}$  in the FTIR spectrum indicated the presence of silicate compounds with Si-O-Si bending vibrations (Saikia and Parthasarathy, 2010). This peak is characteristic of silicate minerals commonly found in soil, such as clay minerals and various crystalline and amorphous silicates. Additionally, the presence of iron oxide minerals, common in soil, can contribute to the observed peaks. Iron oxides, such as hematite and goethite, exhibit vibration modes in the region around 642  $\text{cm}^{-1}$ . The combination of silicate and iron oxide minerals in the soil matrix can lead to overlapping peaks at this wave number in the FTIR spectrum.

While the peak intensity at 775 and 694  $\text{cm}^{-1}$  is decreasing in soil treated with NPK+MN or NPK+MN+herbicides, increased peak intensity was

observed in the soils applied with NPK+FYM and or NPK+FYM+herbicides. This indicates the incorporation of aromatic compounds (Semmler *et al.*, 1991; Karabacak and Kurt, 2009) and their interaction with silicate minerals in soil. Further, the aromatic moieties contained in the herbicides might also interact with organic matter (FYM) and increase the peak intensity. The introduction of aromatic compounds into the soil can have significant implications for various soil functions. Aromatic compounds can influence soil structure and aggregation, thereby affecting the stability of soil aggregates (Aguilera *et al.*, 1997). The presence of these compounds may also enhance the sorption capacity of the soil for other organic pollutants, impacting their mobility and persistence in the environment (Bardi *et al.*, 2000). A shift in peak from 1001 to 996-992  $\text{cm}^{-1}$  was observed due to the application of nutrients, FYM and herbicides. This showed the interaction of silicate clay minerals with micronutrients and polysaccharides from FYM. The presence of this compound in one of the herbicides may interact with organic matter and other soil elements when the herbicide combination is sprayed onto the soil, causing the detection of this specific peak at a particular wave number. This band was broad and strong and covered the area from 1250 to 950  $\text{cm}^{-1}$  (Nuzzo *et al.*, 2020) and represents the Si-O stretching of silicates. While a weak deformation was noticed at 923  $\text{cm}^{-1}$  in MN-applied soil, a small weak absorbance peak was noted at 1515  $\text{cm}^{-1}$  only in the soils treated with FYM. These could be attributed to the deformation of Al-Al-OH bonds and C=C stretching respectively. This showed the presence of aromatic compounds (Krivoshein *et al.*, 2020) in FYM-treated soil since the stretching vibration of carbon-carbon double bonds (C=C) is characteristic of the aromatic rings. Aromatic compounds are molecules containing one or more benzene rings or similar structures.

The appearance and increased absorbance peak intensity over control at 1632  $\text{cm}^{-1}$  and shifting of peak to 1644  $\text{cm}^{-1}$  indicates the deformation of the H-O-H bonds related to the water molecules and the stretching of -C=C- of aliphatic and aromatic groups besides the amide functional groups (C=O-N) originates from FYM and the participation of carbonyl groups on the sorption of applied herbicides particularly the pendimethalin (Ayuba and Nyijime, 2021) and metribuzin. The absorption band at these wave numbers is due to the presence of amide (C=O-N) and aromatic-C=C-stretching vibrations also reported (Du *et al.*, 2014; Krivoshein *et al.*, 2020). However, at this band, a prominent decrease even to negative value was observed in NPK+FYM+herbicides treated soil. It could be attributed to double bond stretching in conjugated or non-conjugated unsaturated compounds and the loss of some unsaturated compounds from the soil (Nuzzo *et al.*, 2020).

Similarly, the NPK+FYM+ herbicides exhibited an additional sharp small absorption peak at 2106-1988  $\text{cm}^{-1}$ , which could be attributed to the carboxylic functional groups added to the soil through FYM and its interaction with herbicides. Peternella and Costa (2021) reported that the absorption band at this wave number could be due to the



CO<sub>2</sub> release during IR measurement by heating and indirectly representing the organic matter presence in soil. The band close to 3630 cm<sup>-1</sup> is due to structural OH groups, particularly to the inner surface of kaolinite minerals in the soil. Intensity at 3612 cm<sup>-1</sup> was sharp and increased for the FYM applied soil beside the peak shifted to 3744-3777 cm<sup>-1</sup> and could be attributed to the OH interaction with organic matter compounds like humic and fulvic acids and involvement in the adsorption of pendimethalin (Ayuba and Nyijime, 2021) and glyphosate.

The overlapping peaks at wave numbers 533, 642, 781, 998 and 1643 cm<sup>-1</sup> were observed in the spectrum and would be assigned to the complexity of the soil matrix. Soil comprises a wide variety of organic and inorganic compounds, each with unique functional groups that can absorb infrared radiation at different frequencies (Smith, 2018). The presence of multiple components with similar or closely spaced absorption bands can lead to peak overlap. Additionally, interactions between the herbicides and nutrient combinations in soil components can create new compounds, further contributing to peak complexity. These interactions may lead to changes in the herbicide degradation rates, transformation products and adsorption capacities, influencing the observed FTIR peak intensities.

#### Assessment of interaction *via* subtraction spectra

A less utilized approach of subtraction spectra was used to identify the exclusive interaction that takes place in soil due to nutrient management practices and herbicide spray. The spectrum of absolute control soil was subtracted from the spectra of treated soil to understand the possible interaction with soil composition. Also, the nutrient practice spectrum was subtracted from their corresponding herbicide-containing spectra to understand the influence of herbicides alone and nutrient management practices alone on their interaction with soil minerals.

Comparison and subtraction of NPK+FYM from NPK+FYM+ herbicides showed that transmittance takes place in soil due to the herbicides (Fig 3). Subtracted spectra show broad stretching band between 3550 to 3150 cm<sup>-1</sup>, a sharp small peak at 2930 cm<sup>-1</sup>, a doublet distinct strong, sharp band between 2250-2400 cm<sup>-1</sup>, a small sharp peak at 1600 cm<sup>-1</sup>, sharp bands at 1200 and 1050 cm<sup>-1</sup>, doublet peak at 800 and 650-700 cm<sup>-1</sup>, sharp strong band at 430-530 cm<sup>-1</sup>. These results showed the strong interaction of NPK+FYM+herbicides in soil and correspondingly brought changes in soil chemical properties both at functional group and fingerprint regions.

The stretching band of 3550 to 3150 cm<sup>-1</sup> and small strong peak at 2930 cm<sup>-1</sup> could be ascribed to the single bond stretching *viz.*, C-H, N-H and C-H present in herbicides as against the weak C-H, N-H stretching alone in NPK+FYM treated soil. The absorption region at 2250-2400 cm<sup>-1</sup> could be assigned to the triple bonds of nitriles and carbenes from applied herbicides. The small sharp peak at 1600 cm<sup>-1</sup> could be assigned to double bonds C=O, C=C and C=N contributed by the added herbicides. The bending vibration bands at 1200 and 1050 cm<sup>-1</sup> could be assigned to C-O, C-C and C-N bonds and at around 800 to 700 cm<sup>-1</sup> to C-C bond and a band between 700 to 400 cm<sup>-1</sup> has been assigned to the minerals in the soil and their interaction with the herbicide composition. Whereas in NPK+FYM, the bands were observed at 2100, 1644 and 1200 cm<sup>-1</sup> only which showed the triple bond carbenes and bending vibrations of C=O and C=N bonds and C-N and C-O only due to the incorporation of FYM. Subtracting the absolute control spectrum from NPK+MN and NPK+MN+ herbicides didn't show much variation. An increased absorption band between 1200 to 1350 and 2114 cm<sup>-1</sup> was noticed in NPK+MN and additionally at 998 cm<sup>-1</sup> in NPK+MN+ herbicides treated soil. These could be ascribed to the N-H stretching from

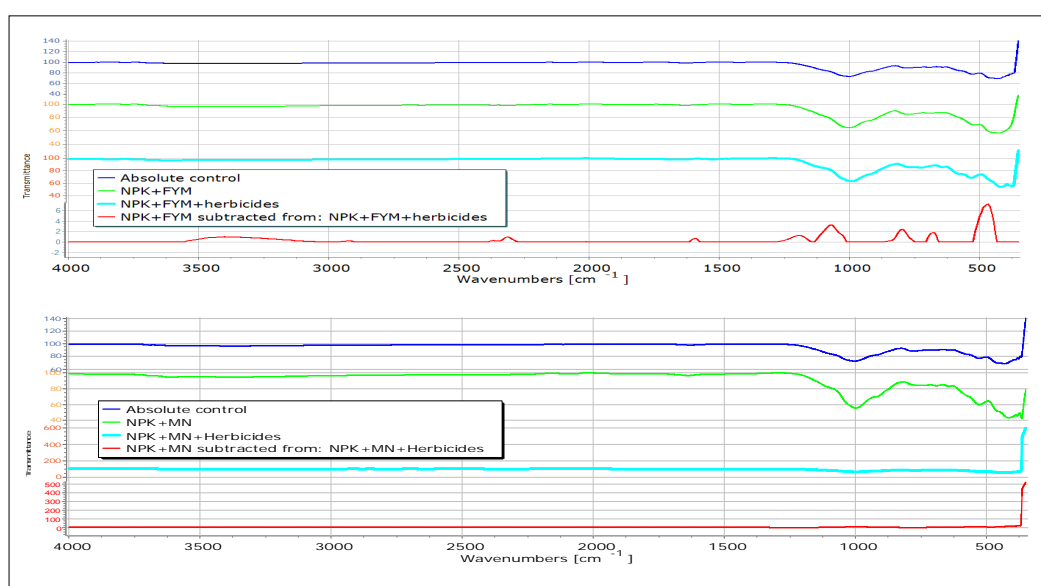
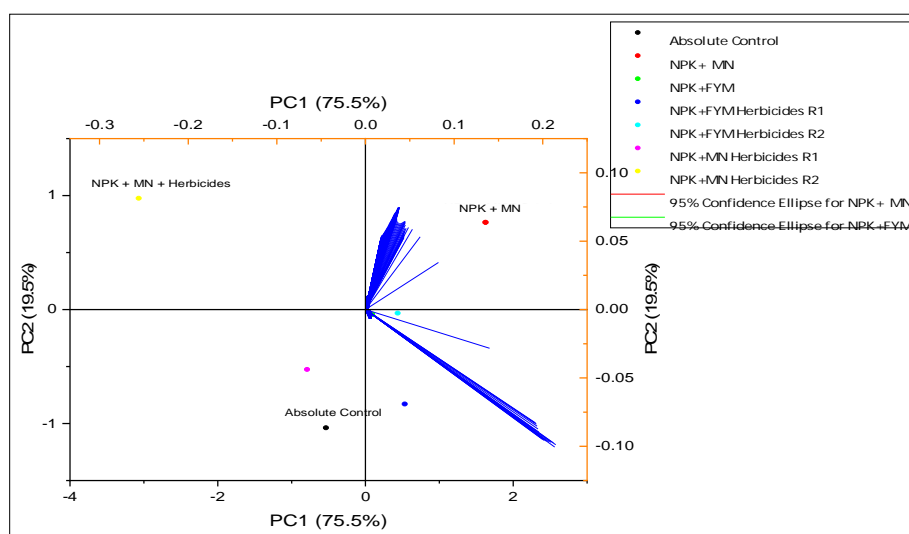


Fig 3: Subtraction spectra of soil treated with herbicides and nutrient management practices.



**Fig 4:** Principal component analysis biplot of the FTIR spectra to understand the contribution of applied herbicides and nutrient management practices' interaction with soil components.

herbicides and the interaction of phosphate-containing glyphosate to the -O-Fe bond in soil (Waiman *et al.*, 2013).

Increased absorption intensity at 998-1004  $\text{cm}^{-1}$  in the treated soils over absolute control could be ascribed to the asymmetric and symmetric vibration of the P-O-Fe bond (Waiman *et al.*, 2013). According to Sheals *et al.* (2002), these bands reflect the formation of monodentate mononuclear inner-sphere complexes, in which the phosphonate moiety is directly bonded to surface Fe (III) centers which are added to the soil through glyphosate or fertilizer or the combination of both in the present study.

#### Principle component analysis (PCA)

The FT - IR data were subjected to principal component analysis (PCA) and the biplot results are presented in Fig 4. Principal component 1 (PC1) and principal component 2 (PC2) explain 75.5% and 19.5% of the total variance of 11 spectroscopic data. For PC1, the main contributing parameters were C=N, C=O, OM-clay mineral bonding and O-Fe complexation with the organic matter and or phosphate molecules originating from the FYM and herbicides. Whereas the PC 2 mainly contributed by the C-H, C-C bonds, stretching O-H bonds of clay minerals (majorly illite and Kaolinite) and other primary minerals like hematite, quartz, *etc.*, were the main contributing parameters for PC2 present in the soil and added through the nutrient fertilizer. The less intensity of absorption at 642  $\text{cm}^{-1}$  and strong negative weightage at 1643  $\text{cm}^{-1}$  in control and MN treated soils and the appearance of additional peaks at 572, 627, 1515, 2108, 2313  $\text{cm}^{-1}$  and increased intensity at 533  $\text{cm}^{-1}$  have contributed to the strong separation of samples into PC1 and PC2, respectively. Similar results were reported for the adsorption of pendimethalin in groundnut hull (Ayuba and Nyijime, 2021) and atrazine in organic soil (Gaffar *et al.*, 2021). The PCA enabled a comprehensive understanding

of the diverse interactions occurring within the soil matrix under different treatments.

#### CONCLUSION

Applied herbicides (glyphosate, pendimethalin and metribuzin) to soils treated with NPK + micronutrients and NPK + FYM revealed intricate and complex interactions, leading to significant changes in FTIR absorption intensities. The presence of observed peaks at varying wave numbers, along with their shifts in the treated soils, provides compelling evidence of specific interactions between the herbicides and the soil inorganic constituents, as well as the organic matter introduced through FYM. These findings underscore the complexity of herbicide-soil interactions in agricultural systems. This research provides insights into optimizing herbicide use and promoting sustainable agriculture practices while showcasing the potential of FTIR spectroscopy in unravelling the intricacies of soil-herbicide interactions.

**Conflict of interest:** None.

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