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Identification of Functional Groups of Rapitest Luster Leaf Products for Soil Phosphorus Testing Based on Color Changes using Fourier Transform Infrared Spectroscopy (FTIR)

Nur Asriyani[1], and Hilda Rahmawati[2]

1. Departement of Physics, Indonesia Defense University, Bogor, Indonesia, 16810
2. Departement of Physics, Cokroaminoto University Palopo, Palopo, Indonesia, 91911

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Abstract

Phosphorus is an important nutrient for plants and is useful as the main driver of primary productivity in plants. Periodic soil phosphorus testing is essential to monitor the availability of phosphorus in the soil so that it is not excessive or reduced to achieve maximum productivity. Testing using laboratory methods takes a long time and is expensive. Rapitest Luster Leaf is a soil testing product based on color changes using a colorimetric method of mixing reagents and color indicators that is practical, easy, portable, and can be used directly on agricultural land. Identification of Rapitest functional groups using FTIR is carried out to predict compound content as a renewable material for soil testing. The analysis showed that the functional groups formed include SO_4^{2}*, which occurs at 987, 631, and 602* cm^{-1} *vibration waves. It indicates that the vibration is shifting to the right. At vibrations of 677-573* cm^{-1}*, the absorption of the* Na_2SO_4 *compound occurs. Sodium sulfate is predicted to be a reagent compound contained in Rapitest. At 811-901 cm-1 and 3524-3209 cm-1 vibration waves, functional group bonds of Mo-O and N-H are formed, respectively. The molecular bonds formed predict that ammonium molybdate is the color indicator compound used.*

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Abstrak

Fosfor merupakan nutrisi penting bagi tanaman berguna sebagai penggerak utama produktivitas primer pada tumbuhan. Pengujian fosfor tanah secara berkala sangat diperlukan guna untuk memantau ketersediaan fosfor pada tanah supaya tidak berlebih atau berkurang untuk mencapai produktivitas yang maksimal. Penggujian menggunakan metode laboratorium memerlukan waktu lama dan biaya yang tinggi. Rapitest Luster Leaf merupakan produk pengujian tanah berbasis perubahan warna dengan menggunakan metode kolorimetri pencampuran antara reagen dan indikator warna yang praktis, mudah, portabel, dan dapat digunakan langsung pada lahan pertanian. Identifikasi gugus fungsi Rapitest dengan menggunakan FTIR dilakukan untuk memprediksi kandungan senyawa, sehingga dapat menjadi renewable materials *untuk pengujian tanah. Hasil analisis menunjukkan bahwa gugus fungsi yang terbentuk diantaranya* SO_4^{2-} *yang terjadi pada vibrasi gelombang 987, 631, 602* cm^{-1} *hal tersebut menunjukkan bahwa vibrasi semakin bergeser kekanan. Pada vibrasi 677-573* cm^{-1} *menunjukkan terjadinya penyerapan senyawa* Na_2SO_4*. Natrium sulfat diprediksi sebagai senyawa reagen yang terkandung pada Rapitest. Pada vibrasi gelombang 811-901* cm^{-1} *dan 3524-3209* cm^{-1} *terbentuk ikatan gugus fungsi masing-masing Mo-O dan N-H. Ikatan molekul yang terbentuk memprediksi bahwa senyawa indikator warna yang digunakan adalah ammonium molibdate.*

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* Corresponding author.
E-mail address: nur.asriyani@idu.ac.id

1. Introduction

Plant nutrient management is essential to maximize crop yields and economic viability. However, improper application can result in decreased crop quality and productivity (Abd El Lateef et al., 2024). Low agricultural productivity is caused by poor agricultural management practices, soil moisture stress, soil degradation, and soil infertility (Ndegwa et al., 2023). Soil fertility is an important factor that directly impacts the performance and quality of crop production. Eleven soil properties, namely electrical conductivity (EC), soil organic carbon (SOC), total nitrogen (TN), calcium carbonate equivalent (CCE), exchangeable potassium (Kex), iron (Fe), copper (Cu), zinc (Zn), manganese (Mn), soil pH, and available phosphorus (Pav) (Zaheri Abdehvand et al., 2024). Phosphorus (P) is an essential nutrient for plants as an important driver of terrestrial primary productivity in all biomes to achieve optimal harvest yields, but excess levels harm crop productivity. (Darela-Filho et al., 2024)(Van Doorn et al., 2024)(Muntwyler et al., 2024). Optimizing the level of phosphorus fertilizer needed is essential to avoid over- and under-use. (Sajindra et al., 2024). The solution to this problem is to periodically test the soil phosphorus content to determine the level of soil phosphorus content and provide appropriate fertilization recommendations based on plant needs. (Pradhan et al., 2020).

Traditional soil measurement using laboratory methods requires expensive laboratory instrumentation and additional extract solutions for further chemical analysis. Although laboratory methods produce accurate analysis, they cannot provide continuous and real-time agricultural analysis. Laboratory methods are constrained by time per sample and cost per sample. So, farmers in large-scale agricultural land areas can only analyze soil using laboratory methods. (Burton et al., 2020). Developing a rapid, accurate, cost-effective soil analysis method for estimating constituents associated with soil phosphorus (P) content is essential. (Mustaqimah et al., 2024).

Sharma and Chatterjee have conducted soil testing based on color changes using Hanna, Hach, LaMotte, and Rapitest products. Hanna, Hach, and LaMotte use colorimeter and turbidimetry methods, while Rapitest only uses the colorimeter method. Rapitest is a soil testing tool that is more practical and cheaper than Hanna, Hach, and LaMotte. The advantage of using the Rapitest is that soil testing can be done on agricultural land (Kihara et al., 2016)(Sharma & Chatterjee, 2019). The Rapitest Luster Leaf product is a soil-testing product based on color changes using the colorimeter method by mixing reagents and color indicators. The test is done by mixing the product with water and soil and observing the resulting color changes. The resulting color changes are matched with color standards that indicate soil content (Asriyani et al., 2022)(Rayment & Lyons, 2011). Rapitest products can only be purchased abroad, and phosphate testing using the Rapitest only produces qualitative data. So, in this study, functional group identification was carried out using FTIR to determine the prediction of compounds in the product so that it can innovate renewable energy for soil phosphorus testing, thus producing more accurate soil testing products in the form of quantitative data.

Fourier Transform Infrared Spectroscopy (FTIR) is well suited to compound conservation due to its flexibility and specificity. With FTIR, it is possible to identify the functional groups of both organic materials, which can be found in compounds in the form of binders, colorants, and surface finishes, as well as inorganic materials (Rosi et al., 2019)(Liu & Kazarian, 2022)(Prati et al., 2016). The fundamental vibration frequency of chemical bonds is usually found in the mid-IR (4000−400 cm−1), a region that is easily accessible with most benchtop FTIR spectrometers, and this will appear in the reflectance or transmission spectrum as a grouping of sharp, well-defined peaks indicating the functional group bonds of the molecules being formed (Diaz-Granados et al., 2024).

Based on the explained background description, the Rapitest Luster Leaf functional group will be identified for testing soil phosphorus content based on color changes using FTIR. This study is expected to identify compounds in the product so that it can innovate to create renewable materials for cheap, practical, efficient, and accurate soil phosphorus testing.

2. Research Methods

This study used the FTIR analysis method to see the functional groups and compounds in the Rapitest Luster Leaf for soil phosphorus testing. The Rapitest Luster Leaf product can be shown in **Figure 1**. The infrared spectrum of the Rapid Test Luster Leaf powder was measured at room temperature by damped total reflectance Fourier transform infrared spectroscopy (ATR-FTIR), using a Bruker vacuum spectrometer, model VERTEX 70 V equipped with an ATR single reflection accessory (Platinum, Bruker Optics), recording a spectral range of 4,000 to 0 cm^{-1} with a resolution of 2 cm^{-1}, accumulating 128 scans based on the spectrum (César Silva et al., 2024). FTIR is a fundamental analytical technique across scientific domains, facilitating comprehensive analysis of molecular structures and functional groups in various compounds. Through measuring the absorption of infrared radiation, FTIR spectroscopy enables the identification of characteristic absorption peaks, revealing the specific functional groups present in a sample (Md Siddique, 2024).

FTIR spectroscopy, accompanied by quantum chemical simulations, can reveal important information about the molecular structure and intermolecular interactions in the condensed phase (Le et al., 2024). FTIR is based on atomic vibrations and rotations and has become a universal and widely used spectral methodology for detecting internal molecular structures in all types of materials (Gong et al., 2024). An illustration of the Fourier transform infrared spectrometer is shown in **Figure 2**. Fourier transform infrared spectrometer FTIR results can be analyzed using origin to determine the peak of the vibration spectrum produced in the spectrum range of 4000-400 cm^{-1}. The vibration peak at a certain wave energy will produce different atomic bond groups. The bond groups formed can be seen through previous research journal references.

Figure 1. Rapitest Luster Leaf.

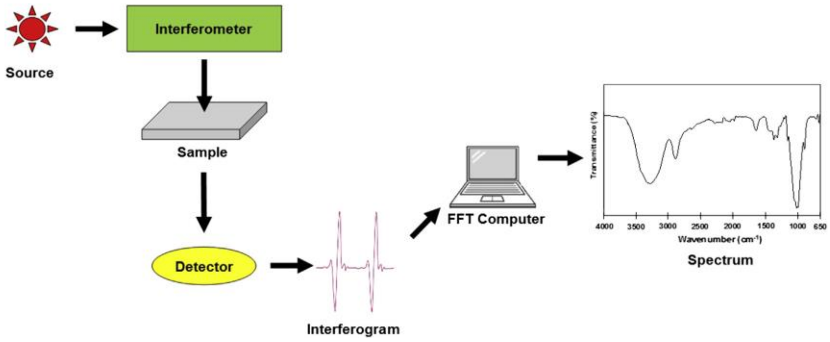


Figure 2. Illustration of a Fourier transform infrared spectrometer (Mohamed et al., 2017).

3. Results and Discussions

Functional group vibrations in Rapitest Luster Leaf products for soil phosphorus testing can be analyzed using FTIR. **Figure 3** shows the FTIR spectrum of soil phosphorus testing products with variations in the increase in reagent manufacturing temperature. The absorption curvature indicates the level of potential energy and force constant. The deeper the curvature, the greater the level of potential bond energy and force constant (Nakamto, 1979). The functional groups formed in the Soil Test Kit phosphorus product are shown in **Table 1.** The results of the soil phosphorus test product's spectrum have similarities with the sulfate ion vibration reference. However, the reference results do not indicate the content of potassium hydroxide tetrahydrate. The spectrum results indicate the presence of sulfate ion functional groups. The sulfate ion functional group has four vibration modes, including non-degenerate mode (υ_1), double degenerate mode (υ_2), and triple degenerate mode ($\upsilon 3$ and $\upsilon 4$)(Prameena et al., 2013).

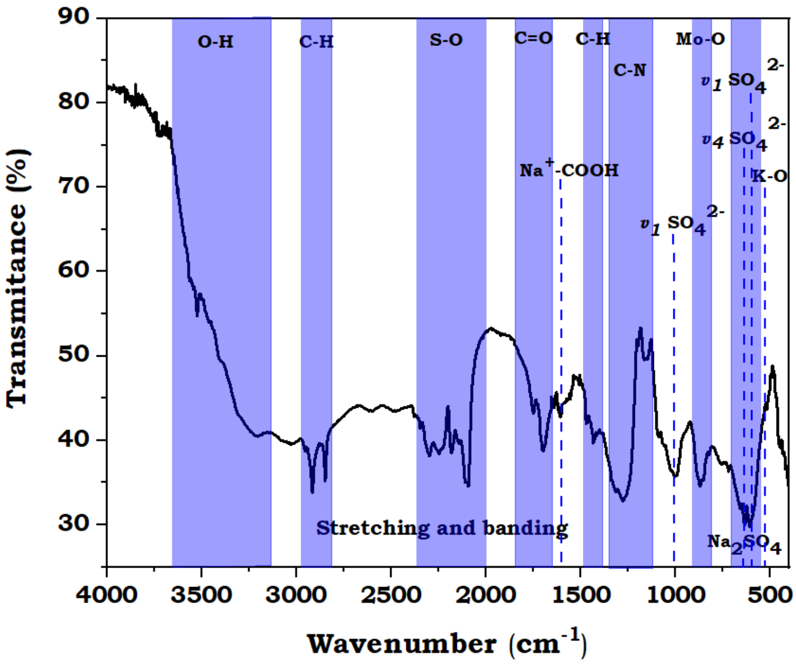
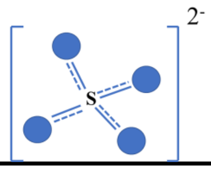
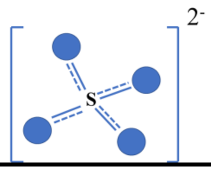
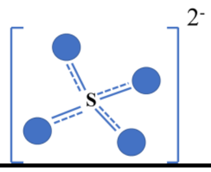
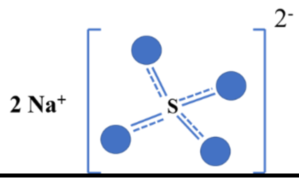


Figure 3. FTIR spectrum results on Rapid Test Luster Leaf for soil phosphorus testing.

Table 1. FTIR spectrum results on Rapitest Luster Leaf for soil phosphorus testing.

Wavenumber (Cm^{-1})	**Functional groups**	**Vibration Mode**	**Atomic Structure**
553 (Theodosoglou et al., 2017)	K-O	-	**K—O**
602 (Tang et al., 2020)(Akash & Rehman, 2019)(James & Wood, 1925)	SO_4^{2-}	υ_1	
631 (Tang et al., 2020)(Akash & Rehman, 2019)(James & Wood, 1925)	SO_4^{2-}	υ_4	
987 (Tang et al., 2020)(Akash & Rehman, 2019)(K. Sharma et al., 2018)(Santus, 2020)	SO_4^{2-}	υ_1	
677-573 (Stenger et al., 2010)	Na_2SO_4	-	
1139-1134; 1340-1250 (Coates, 2006)	C-N	-	**C—N**
811-901 (Ren et al., 2024)	Mo-O	-	**Mo— O**
1500-1387 (Nandiyanto et al., 2019)	C-H	-	**C—H**
1602 (Daemi & Barikani, 2012)	Na^+-COOH	-	**Na^+— COOH**
1791 dan 1653 (Kinoshita, 1990)	C=O	-	**C=O**
Sekitar 2000 (Dabhade et al., 2009)(Nakamto, 1979)	S-O	*Stretching* dan *banding*	**S—O**
3524-3209(Khodiev et al., 2023)	N-H	-	**O—H**

The absorption centered at 987 cm^{-1} causes asymmetric strain vibrations of the SO_4^{2-} functional group, resulting in vibrations with a non-degenerate mode (υ_1) (Tang et al., 2020)(Akash & Rehman, 2019) (K. Sharma et al., 2018)(Santus, 2020). At the absorption peak centered at 631 cm^{-1}, SO_4^{2-} vibrations occur with a three-degenerate mode (υ_4), and at 602 cm^{-1}, SO_4^{2-} vibrations occur with a nondegenerate mode (υ_1) (Tang et al., 2020)(Akash & Rehman, 2019)(James & Wood, 1925). The peak around 677-573 cm^{-1} is the spectrum of sodium sulfate, which indicates the occurrence of a photochemical reaction involving the cleavage of the sulfonate group on the organic anion and the formation of sodium sulfate (Na_2SO_4) (Stenger et al., 2010). At the peak around 2000 cm^{-1}, stretching and banding occur in the sulfur-oxygen (S-O) functional group (Dabhade et al., 2009)(Nakamto, 1979). Based on the results of functional group analysis, the reagent compound contained in Rapitest is sodium sulfate.

At vibration 1602 cm^{-1}, asymmetric stretching vibrations occur from the carboxylate group, resulting in regular homopolymer chain interactions with sodium ions (Na^+-COOH) (Daemi & Barikani, 2012). At Sample 1791 and 1653 cm^{-1} peaks, vibrations of the C=O functional group occur (Kinoshita, 1990). The C-H functional group occurs when asymmetric stretching vibrations occur at 1500-1387 cm^{-1} (Nandiyanto et al., 2019). The C=O and C-H functional groups decrease with increasing temperature in the reagent preparation. The vibrations around 3311 cm^{-1} are caused by antisymmetric stretching vibrations of H_2O molecules related to the increasing intensity of alkali metal activity. The position of this band is formed by intermolecular H bonds formed by O-H groups after KOH treatment. So, the vibration at around 553 cm^{-1} results in stretching the K-O vibration (Theodosoglou et al., 2017). The vibrations around 811-901 cm^{-1} indicate that there is absorption of the Mo-O functional group(Ren et al., 2024). The N-H stretching frequency is located in the 3524-3209 cm^{-1}, then shifts to the region of 3209 cm^{-1} (Khodiev et al., 2023). The Mo-O functional group is related to the N-H bond. The predicted color indicator contained in Rapitest for soil phosphorus testing is ammonium molybdate.

Based on the functional group analysis and assessment results, sodium sulfate (Na_2SO_4) is the reagent material used. Based on the functional group analysis results, the reagent is obtained from the mixing reaction between potassium sulfate and sodium hydroxide to produce sodium sulfate and potassium hydroxide. This reaction is an ionic reaction. The chemical reaction of sodium sulfate is depicted in **Figure 4**. **Figure 5** shows the reaction mechanism of sodium sulfate with soil solution. The color indicator used uses ammonium molybdate. Sodium sulfate will bind phosphate ions in the soil, causing a color change. The resulting color change indicates the soil's phosphorus content level (Mohammadkhani et al., 2011). The predicted material can provide material innovation for color change-based soil phosphorus testing with test results in the form of more accurate quantitative data on a percentage scale.

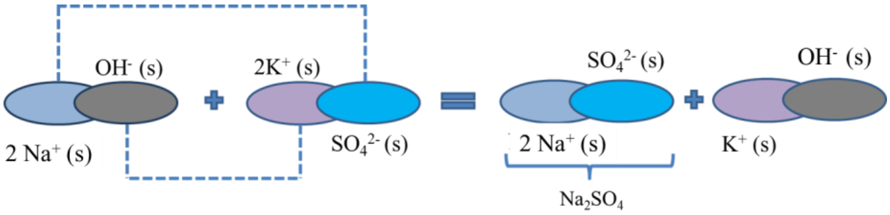


Figure 4. Reaction for the formation of soil phosphorus test products.

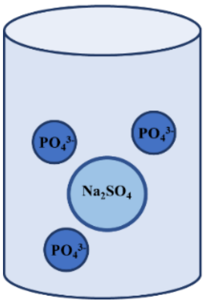


Figure 5. Reaction mechanism of sodium sulfate with soil solution.

4. Conclusions

Rapitest Luster Leaf is formed from a mixture of reagents and color indicators. Based on the results of FTIR analysis on the Rapitest Luster Leaf product, the functional groups formed include SO_4^{2-} which occurs at vibration waves of 987, 631, and 602 cm^{-1}. It indicates that the vibration is shifting to the right. At vibrations of 677-573 cm^{-1}, the absorption of the Na_2SO_4 compound occurs. Sodium sulfate is predicted to be a reagent compound contained in Rapitest. At vibration waves of 811-901 cm^{-1} and 3524-3209 cm^{-1}, bonds of functional groups are formed, namely Mo-O and N-H. The molecular bonds formed predict that ammonium molybdate is the color indicator compound used.

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