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Investigation of Optical Properties of Fluorspar Using XRF, UV-Vis and FTIR Spectrometry

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ABSTRACT
Recently, the Nigerian Senate passed a Bill mandating 30% utilization of all mineral resources in the country before their export. This has attracted more attention to critically examine the structure and properties of the available minerals in Nigeria. In this research, the optical properties of fluorspar have been investigated using different analytical tools such as XRF, UV-Vis and FTIR. The XRF result reveals the presence of rare earth elements; Ce and Dy which may occur as substitutes for Ca in the CaF_2 crystal structure due to their atomic sizes. These were found responsible for causing the fluorite's fluorescence in different colours. The UV-Vis result has shown that absorption peaks at 225 nm and 370 nm were key aspects of fluorite's absorption characteristics. These were not expected to have had impact on the colour of the fluorspar. However, these may be linked to electronic transitions and defects within the crystal structure, which determine how fluorite absorbs light across different wavelengths. Furthermore, these peaks were specifically attributed to electrons and holes trapped in the Ca^{2+} interstitial and vacancy, respectively. The FTIR analysis revealed absorption bands corresponding to CO_2 and CO_3^{2-} stretching vibrations from $CaCO_3$, as well as OH stretching vibrations due to water presence in the samples. The study shows a clear effect of these impurities or inclusions on the fluorspar optical performance.

CITATION
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INTRODUCTION

Fluorspar, also known as fluorite, is known for its amazing optical properties leading to important applications in various industries. It is basically a calcium fluoride (CaF_2) compound, and a naturally occurring mineral that displays a range of vibrant colours, most commonly light to dark blue, but also red, purple, yellow, green, and white. In its purest form, fluorite is colourless (Balogun et al., 1996; Akhter et al., 2018). This mineral is also known to exhibit fluorescence when exposed to cathode-ray and ultraviolet irradiation (Ge et al., 2022). Its optical properties make it super useful in lenses, especially for ultraviolet light applications. For instance, fluorite lenses are used in microscopy and telescopes because they allow for high-resolution images with minimal chromatic aberration (Schumann, 1896). In terms of specific optical properties, fluorite has a refractive index of around 1.433 to 1.448, which is pretty unique. It is also isotropic, meaning its optical properties are the same in all directions (Emsley, 1991). Fuerthermore, fluorite has a high transparency to ultraviolet light, making it perfect for applications like fluorescence microscopy (Polymeris et al., 2006). The colour of fluorite can vary due to impurities, and this affects its optical properties too. For example, rare-earth elements like Eu, Pr, Dy, Tb, Er, and Sm can cause fluorite to fluoresce in different colours, including blue, yellow, green, and red (Öztürk, 2019). Additionally, fluorite's optical properties have been studied in the context of its potential applications in photonics and optoelectronics (Kumar et al., 2018). Researchers have also explored the

use of fluorite in laser technology, highlighting its high damage threshold and low nonlinear refractive index (Miranda et al., 2020). Furthermore, the temperature sensing properties of fluorite have been investigated, finding it remains stable up to 543 K (Bonewitz, 2012). Fluorspar has a face-centered cubic lattice structure (Figure 1).

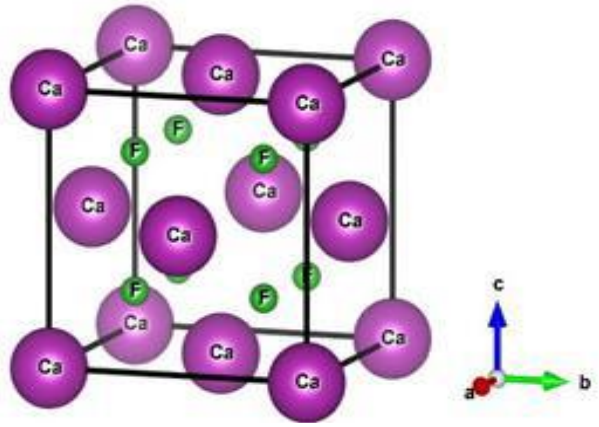

Figure 1: Structure of Fluorspar (Gidado and Ibrahim, 2023)

MATERIALS AND METHODS

To properly investigate the properties of fluorspar properties in the Nigeria (Yantuwaru mining site, Faskari), three (3) analytical methods, UV-Vis, FTIR and XRF were used to analyze the sampled minerals.

Sampling location and procedure

Yantuwaru mining site (Fig. 2) is located within Ruwan-godiya ward, faskari local government area of Katsina State. It is found within the coordinates 11˚45'33"N 7˚12'53.8"E (http://www.mindat.org).

Four distinct coloured fluorspar samples (labelled A, B, E, and J) were considered.

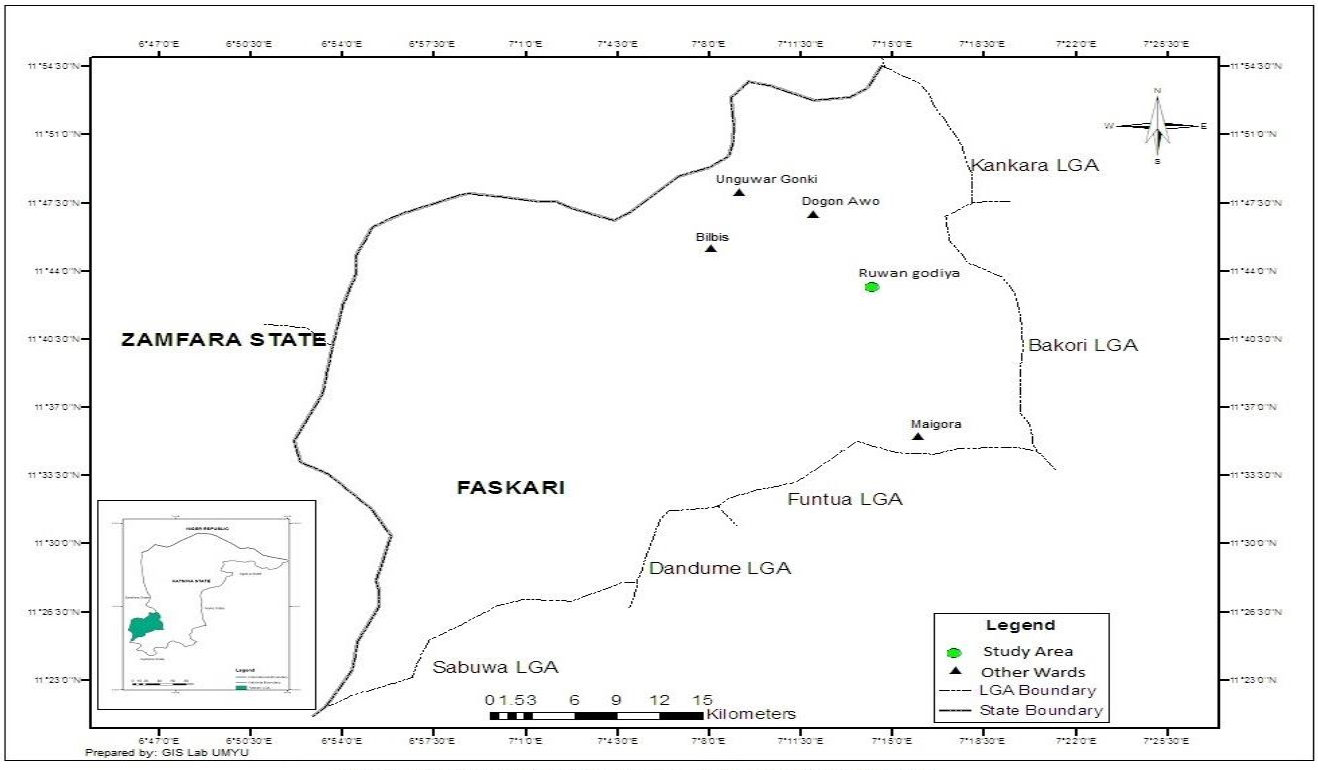

Figure 2: Map of Faskari Local Government Showing the Study Area

The collected fluorspar samples were inserted into some separate pure polyethylene sample containers and transported to the central research laboratory, Umaru Musa Yar'adua University, Katsina for various analyses. The samples were then grinded into fine powder after they were washed with distilled water to remove any attachments.

Figure 3: A fluorspar sample

Figure 4: Yantuwaru mining site (a Fluorspar mining site)

Table 1: Colours for the sampled fluorites collected at Yantuwaru mining site, Ruwan-Godiya Ward, Faskari Local Government, Katsina

S/N	Fluorspar Sample	Fluorspar samples Colour
1	A	Bluish-green
2	B	Green
3	E	Black with a red edge
4	J	Black with partial light-purple coloring.

UV-Vis, FTIR and XRF Analyses

The model AUV-6300PC Double Beam Spectrophotometer UV-Vis available at the Central laboratory was used in this work to analyzed the collected sample. Furthermore, the reflection method was used as the experimental test technique within the 200–900nm scan range at the scan step of 5.0 nm as well as filter precision of 5, in accordance with the literature guide.

The FTIR analysis was also performed on our samples. The Fourier infrared spectrometer by Agilent Technologies was used for the infrared spectra test. Transmission method was adopted under the following experimental test conditions:

Test voltage was 220V, the resolution was 16cm^{-1}, and the scanning range was 4000–650cm^{-1}. This analysis was carried out at the central laboratory, Umaru Musa Yar'adua University, Katsina.

The sampled fluorites were also subjected for XRF analysis for elemental concentrations. The XRF machine available in the same Central Laboratory, Umaru Musa Yaradua University, Katsina, was used for this purpose.

RESULTS AND DISCUSSION

The results for the XRF analysis are presented in Table 2 and 3 in this work. A closer look of Table 2 will show that various elemental compositions and concentrations are available in the analyzed fluorspars. The present work has found a sample of the fluorspar with a very high concentration of Ca (459.55 mg/g) relative a literature (Mangala and Patel, 1996) value which reported a concentration of (166 ± 11 mg/g) in their work. This may due to difference in the fluorite colour. Other values of noticeable concentrations in this work include Cr (165.5 µg/g), Cu (133.87 µg/g), Sr (287.5 µg/g), Yb (58.59 µg/g), Nb (102.05 µg/g) and Pb (148.27 µg/g) which were previously obtained as 76.1 ± 18 µg/g, 30.2 ± 3.8 µg/g, 105 ±7 µg/g, 20.1 ± 1.4 µg/g, 6.5 ± 0.5 µg/g and 65.4 ± 6 µg/g respectively. However, there is less concentration of each of the elements; K (0.423 mg/g), Ti (0.0249 mg/g), Mn (152.35 µg/g), Fe (0.47 mg/g), Zn (25.2 µg/g), Ga (0.41 µg/g), Br (1.62 µg/g), Rb (0.2025 µg/g), and Zr (135.1 µg/g).

Table 2: Elemental content analysis of natural fluorite using X-ray fluorescence

Element	This work (mg/g)	Literature (Mangala and Patel, 1996)
K	0.423*	12.4 ± 0.9*
Ca	459.55*	166 ± 11*
Ti	0.0249*	2.9 ± 0.2*
Cr	165.5	76.1 ± 18
Mn	152.35	584 ± 47
Fe	0.472*	25.4 ± 1.6*
Cu	133.87	30.2 ± 3.8
Zn	25.2	104 ± 7
Ga	0.41	8.6 ± 1.7
Br	1.62	6.8 ± 0.7
Rb	0.2025	48.4 ± 3.1
Sr	287.5	105 ±7
Y	58.59	20.1 ± 1.4
Zr	135.1	183 ± 11
Nb	102.05	6.5 ± 0.5
Pb	148.27	65.4 ± 6

Table 3: Elemental content analysis of natural fluorite using X-ray fluorescence

Elements	This work (ppm)	Literature (Balogun et al., 1996)
Au	ND	56.83 ± 5.87
Ce	8218.3	63.9 ± 7
Co	25.1	12.23 ± 7.25
Dy	0.1	4.2 ± 16
Eu	ND	0.49 ± 12
Hf	11.5	13.61 ± 5.97
La	ND	30.26 ± 1.8
Mn	152.4	611.39 ± 5.2
Sb	ND	2.63 ± 4.9
Sc	665.7	12.5 + 0.94
Sm	ND	15.94 ± 0.37
Ta	357.3	0.86 ± 9.6
Tb	ND	0.33 ± 12.96
Th	0.04	8.9 ± 2.79
V	4.0	61.38 ± 13.8
Yb	ND	1.76 ± 6.94

Key ND: Not Detected

Table 3 compares the values of some elemental concentration in this work with another work in the literature (Balogun et al., 1996). Several elements were not detected. These elements include; Au, Eu, La, Sb, Sm, Tb and Yb. The vanadium (V) (4.0 ppm) was found here in our work as a trace concentration but with higher reported value in the literature (Balogun et al., 1996), having 61.38 ± 13.8 ppm. The elements; Ce (8218.3 ppm) and Hf (11.5 ppm) had concentrations 63.9 ± 7 ppm and 13.61 ± 5.97 ppm in (Balogun, 1996) also as minor elements. Similarly, Th (0.04 ppm) and Dy (0.1 ppm) have been reported in this study, in contrast to the reported literature (Balogun et al., 1996) trace data of 8.9 ± 2.79 and 4.2 ± 16 respectively. The rare earth elements; Ce and Dy may occur as substitutes for Ca in the CaF_2 crystal structure due to their atomic sizes.

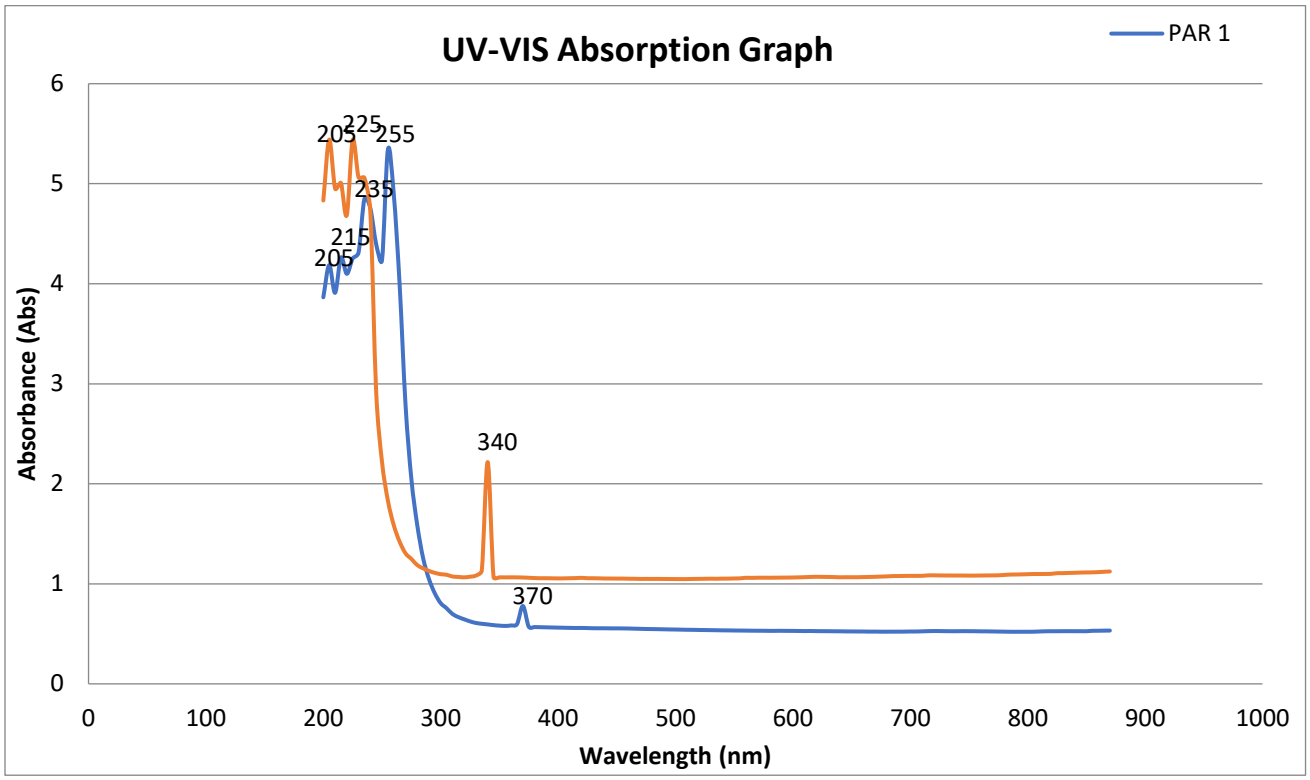

Figure 5: UV-Vis Spectra for two (2) different fluorite samples

The UV-Vis result has been presented in Fig. 5. Both samples display absorption peaks between 205-370 nm, which might be linked to impurity ion crystal field or charge transfer peaks (Bill, 1982; Scouler, 1960). This did not cause exhibition of any colours due to fluorite's high transparency to ultraviolet light suggesting its good transmittance in the UV range. These absorption peaks at specific wavelengths (between 205 nm to 370 nm) may not necessarily impact the fluorite's colour (Ge et al., 2022). However, both samples has shown no absorbance in the visible range owing to this transmission level (Bill & Calas, 1978; Mitra, 1981). The absorption bands near 224 nm (225nm specifically) were caused by electrons trapped in Ca^{2+} interstitials, while those near 365 nm (370 nm specifically) were caused by holes trapped in Ca^{2+} vacancies (Kim et al., 2013; Wenjun, 1999). This may also be related to Ce^{3+} (Mitra, 1981)due to energy from the light is being absorbed by the electrons and holes trapped in Ca^{2+} interstitials and vacancies. The fluorite's refractive index and its isotropic nature might influence the reflectance property of fluorspar. This isotropic nature ensures consistent reflectance properties, which is useful in optical applications.

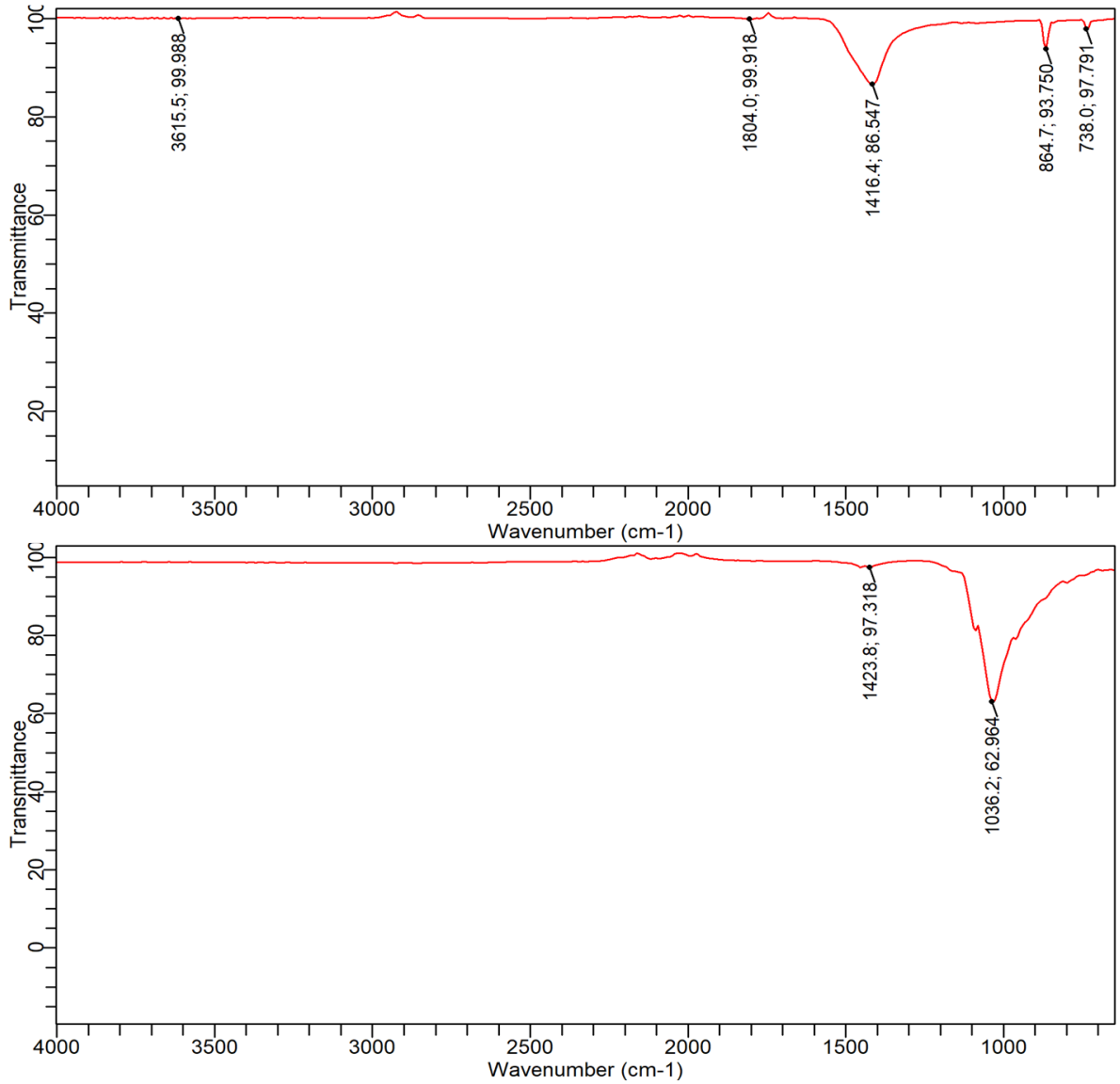

Figure 6: FTIR results of the four analyzed samples

In Fig. 6, the FTIR results of the four (4) analyzed samples have been presented. The Fig. is a representation of the infrared spectra of the four samples of fluorspar. The FTIR spectra of fluorite samples exhibit a broad absorption band around 1050 cm^{-1}, which is a characteristic feature of CaF_2 and aligns with the mineral spectroscopy peaks at 1080 and 1110 cm^{-1} (Zongming, 1990; Ge et al., 2022). The Fig. shows peaks at 1450 and 1650 cm^{-1}, which are attributed to the CO_3^{2-} stretching vibrations, indicating the presence of $CaCO_3$ (Ge et al., 2022; Garrido-Cordero et al., 2020; Jia et al., 2019; Li et al., 2017). Additionally, peaks at 2000, 2100, and 2300 cm^{-1} are likely caused by the inclusion of CO_2 within the fluorite samples (Ge et al., 2022; Megasari et al., 2018). The absorption peak at 2875 cm^{-1} results in the adsorption of oleic acid ester on the fluorspar surface is associated with organic groups (Zhifeng& Hong, 2015). Furthermore, the characteristic peak at 3370 cm^{-1} is due to OH stretching vibration, suggesting the presence of constitutional water in fluorite, a phenomenon also observed in fluorite samples from China, India, and Mexico (Ge et al., 2022; Singh, 2013; Baatartsogt et al., 2007).

CONCLUSION

The XRF analysis confirmed the presence of few rare-earth elements as impurities which might be responsible for the fluorite to absorb light and fluoresce in different colours. The UV-Visible absorption peaks at 224nm and 365nm, are key aspects of fluorite's optical properties. These absorption peaks are linked to the electronic transitions and defects within the crystal structure, which influence fluorite's optical behavior by determining how it absorbs and transmits light across different wavelengths. This means that the fluorspar will absorb light more strongly at certain specific wavelengths thereby affecting its transparency, fluorescence and other optical

performance. The absorption at these peaks can lead to fluorite appearing coloured or fluorescing under certain lighting conditions. The electronic transitions and defects within the crystal structure are the underlying causes of these absorption peaks, directly shaping how fluorite interacts with light.

The FTIR results, on the other hand, shows absorptions due to CO_2, CO_3^{2-} and OH stretching vibrations. This gives a clear picture of the sample's optical properties by revealing the presence of CO_2, CO_3^{2-} and OH as impurities or inclusions that affect its optical performance.

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