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Nada Falih M

Mithaq M. Mahdy AL-Sultani

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Chemical Structure and Optical Properties of Calcium Oxalate Human Kidney Stones

Nada F. Mahdi*, Mithaq M. Al-Sultani

Department of Physics, College of Education for Girls, University of Kufa, Najaf, Iraq

Abstract

The research aimed to study the components and optical properties of ten calcium oxalate human kidney stones in Al-Sader Medical City in the city of Najaf. The FTIR analyzer for all stone samples was investigated by Bruker Alpha II Fourier transform infrared spectrometer with a Spectral range of 375–7500 cm^{-1}. The result shows that every stone sample consists of components like whewellite, weddellite, uric acid, ammonium urate, and carbonate apatite. Still, the highest percentages of the components of the stones are calcium oxalate. The optical absorbance, transmittance, reflectance, and absorption coefficient for all stones were investigated. The result shows the highest absorbance in sample 10, while the values of the absorption coefficient increase with the increase of uric acid content in calcium oxalate stones.

Keywords: Kidney stones, Calcium oxalate stone, Chemical structure, Optical properties

1. Introduction

The prevalence of urinary stone disease remains significant on a global scale, with kidney stones representing a prevalent and distressing condition within the urinary system [1]. Urinary calculi, referred to as kidney/ureter/bladder/urethra calculus or uroliths, are crystalline deposits that form within the urinary system. The ailment, as mentioned above elicits intense acute discomfort and pain in the sufferer. Urinary calculus disease ranks as the third most prevalent area within the field of urology, following urinary tract infection and prostate disease, as determined by patient population [2]. Kidney stone disease affects ~10% of the United States population and about 50 million people in the world [3]. The prevalence of this condition is observed to be increasing, with approximately 7% of women and 12% of men experiencing its effects throughout their lifetimes [4]. The development of kidney stones is an intricate and multifaceted phenomenon that involves various elements, both inherent (such as age, gender, and genetic predisposition) and external, including geographical location, climate, dietary habits, mineral composition, and water consumption [5]. The chemical phenomena of nucleation and crystal growth play a crucial role in the commencement and progression of various stone formations. The initial phase of the crystallization process involves nucleation, wherein solute molecules scattered within a solvent start to aggregate, either through homogeneous or heterogeneous means. The aforementioned process can occur when particles composed of proteins, other organic polymers, or crystals of a different mineral are present. Furthermore, this activity is confined within receptacles lined with chemically active cell surfaces [6]. In the context of a supersaturated liquid, cluster formation occurs when free atoms, ions, or molecules aggregate into small-scale structures. These clusters subsequently undergo precipitation when their overall free energy decreases than the surrounding liquid slower lower than the surrounding liquid.

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* Corresponding author.
E-mail address: nadaf.almudhafar51@student.uokufa.edu.iq (N.F. Mahdi).

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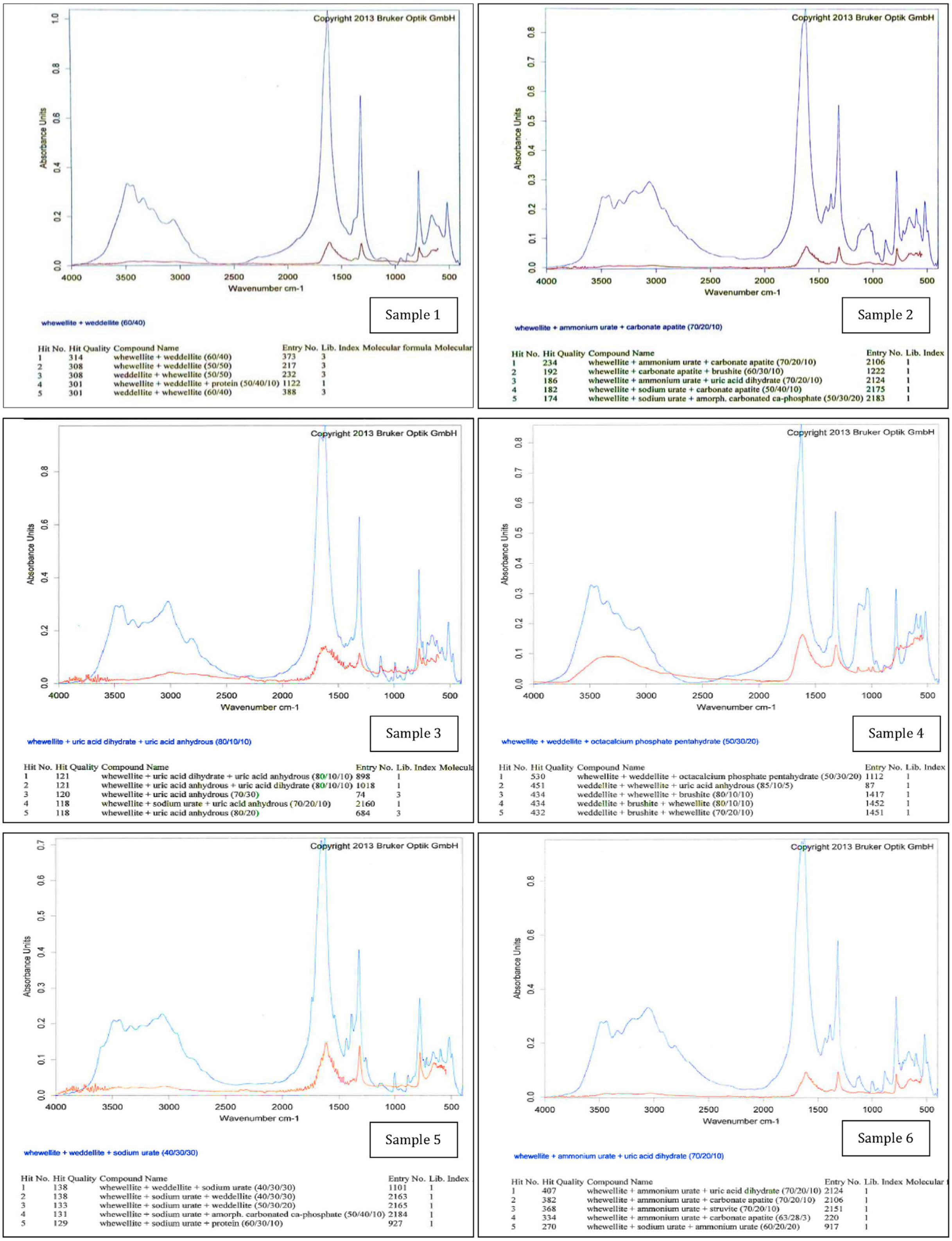

Fig. 1 The FTIR analyzer of stone samples.

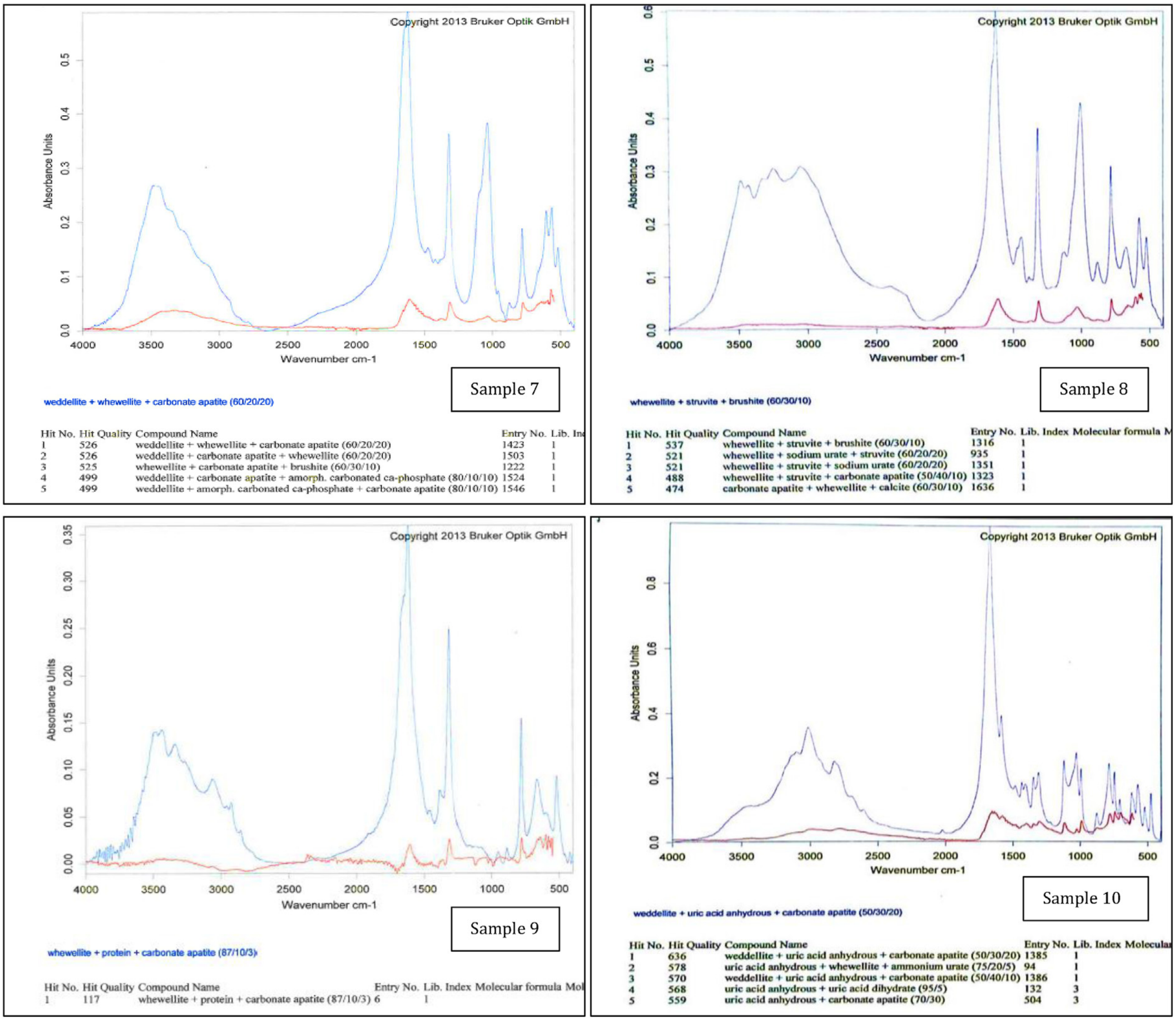

Fig. 1 (Continued).

The aggregation of crystals in urine results in the formation of a compact concretion known as crystal growth. The process of stone growth involves the agglomeration of preexisting crystals or the subsequent nucleation of crystals on a surface coated with a matrix. The phenomenon of stone growth is characterized by a gradual and protracted progression, necessitating an extended duration to impede the functionality of the renal tubules [7].

Multiple classifications of urinary tract stones exist, which are determined by the composition of crystals or chemicals comprising them [1]. Uric acid stones account for around 8–10% of the total prevalence of kidney stones on a global scale. Struvite stones, sometimes called "infection stones," account for approximately 7–8% of the total stones found globally [6,8,9]. Calcium stones are the prevailing type of renal stones, accounting for approximately 80% of all urinary calculi [5]. The majority of kidney stones consist predominantly of calcium oxalate (CaOx), which can occur in the form of either a monohydrate or dihydrate. The CaOx monohydrate (whewellite, COM) crystals exhibit a thin and plate-like morphology, often assuming a twinned structure resembling a 'dumb-bell' form, as observed in urine sediments. Crystals of calcium oxalate dihydrate (known as weddellite or COD) exhibit a distinctive tetragonal bipyramidal morphology, which is observed in both urine sediment and kidney stones. The prevalence of COM stones surpasses that of pure COD stones. Calcium phosphate (CaP) is primarily encountered in the form of basic CaP (apatite), calcium hydrogen phosphate dihydrate (brushite), or tricalcium phosphate (whitlockite). The occurrence of pure calcium phosphate (CaP) stones is infrequent [6,7,10]. CaOx stone formation is primarily facilitated by the presence of specific proteins inside the organic matrix, namely

Tamm-Horsfall protein and osteopontin. The process of crystal aggregation is often regarded as the pivotal stage in the production of stones, wherein a minute solid crystal in a solution adheres to others, resulting in the formation of a bigger stone [7].

2. Get rid of kidney stone methods

The formation of urinary and kidney stones occurs as a consequence of the precipitation of dissolved salts in the urine. These conditions are associated with discomfort and necessitate certain medical interventions for resolution. Stones with a diameter of $\leq$4 mm typically exhibit a propensity for spontaneous passage, obviating the need for surgical intervention. Alternative approaches may be employed in such cases [11]. The presence of kidney stones is constantly linked to lifestyle factors such as being overweight and experiencing weight increases. Therefore, it is necessary to focus on weight management not only to avoid the occurrence of kidney stones but also to reduce the progression of related co-morbidities. Moreover, it is widely acknowledged that fluid treatment plays a crucial role in promoting an augmented urine volume by augmentation fluid consumption. The advantageous outcome was illustrated in a single randomized experiment that examined the occurrences of kidney stone recurrences [12]. The pharmacological treatment presents an alternative approach to stone elimination. However, it is advisable to limit the administration of medications to those with moderate to severe stone disease who have not responded to conservative interventions involving dietary adjustments and increased fluid consumption [13]. In cases where a kidney stone fails to pass or relocate within a clinically reasonable timeframe of approximately 30 days and afterward induces persistent, severe, and unrelenting pain, urological treatments may be deemed necessary for its removal [1]. The holmium: yttrium aluminum garnet (Ho: YAG) laser has been widely utilized for lithotripsy for a period exceeding two decades [14]. The flashlamp-pumped, solid-state, long-pulse, Holmium:YAG infrared laser represents a notable advancement in the field of urology laser technology. The clinical utilization of the Ho: YAG laser for lithotripsy commenced in 1993, although investigations pertaining to this technology date back to the 1990s. The holmium wavelength is highly suitable for intracorporal/endoscopic lithotripsy owing to its efficient transmission through optical fibers [15].

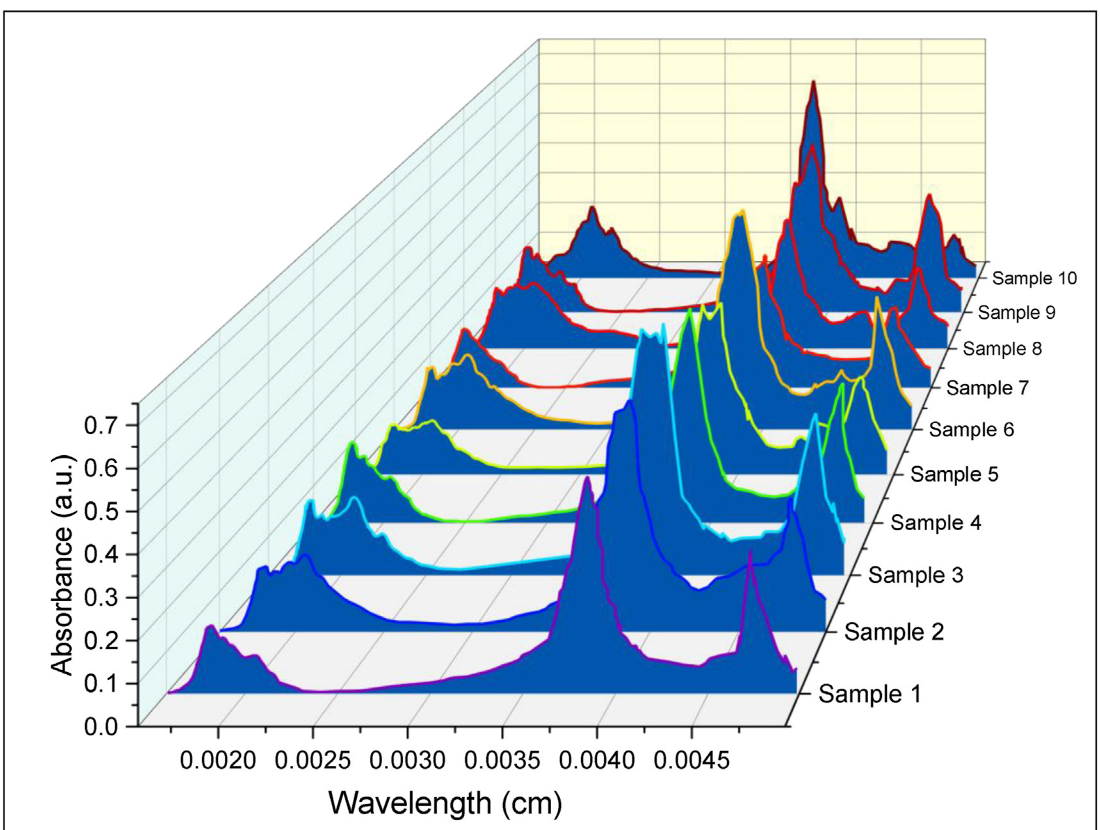

Fig. 2. Optical absorbance spectra of the calcium oxalate stone for samples.

3. The interaction of light with tissue

There are four primary manners in which light may interact with tissue: transmission, reflection, scattering, and absorption [16]. The absorption coefficient, denoted as $\mu_a(\lambda)$, characterizes the reduction in intensity of light as it is through a stone. The concept can be interpreted as the aggregate of the absorption cross-sections per unit volume of a stone with respect to an optical phenomenon [17]. The absorption coefficient $\mu_a(\lambda)$ can be given by [17,18]:

$$\mu_a(\lambda) = \frac{2.303 * A}{d} \quad (1)$$

Where d is the thickness of the stone, a the absorbance can define as the ratio of the absorbed intensity I_A and the incoming one [19]:

$$A = \frac{I_A}{I_0} \quad (2)$$

The ratio (I/I_0) is known as transmittance (T), which is the ratio between the intensity of the transmitting light ray to the intensity of the incident ray [20], is given by the following relationship [17,21]:

$$T = e^{-\mu_a(\lambda) d} \quad (3)$$

In the presence of absorbance and scatter, the energy conservation law may be written as [19].

$$T + R + A + S = 1 \quad (4)$$

4. Materials and methods

Ten stone samples of calcium oxalate have been collected from Al- Sader Medical City in Najaf. A small part of the stone was cut and ground into a powder to prepare it for the FTIR analyzer. Bruker Alpha II Fourier investigated the FTIR analyzer for all stone samples transform infrared spectrometer with a spectral range of 375—7500 cm^{-1}, and spectral resolution better than 2 cm^{-1} is used to identify functional groups in organic molecules of stones. The optical properties were studied through the absorbance extracted from the FTIR analyzer.

5. Results and discussion

Figure 1 shows the FTIR analyzer for all stone samples. The absorbance-wavenumber spectra depend on the chemical structure of the stones. The

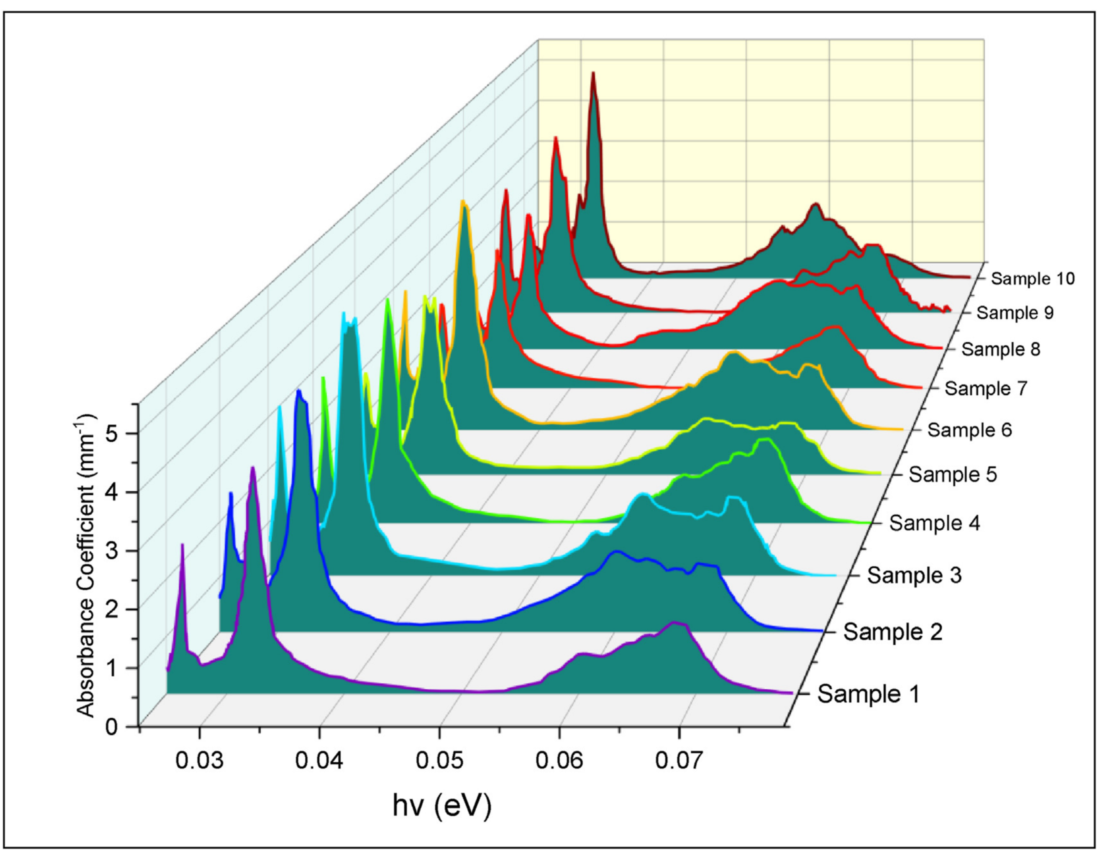

Fig. 3. Optical absorbance coefficient of the calcium oxalate stone for samples.

fundamental peak was shifted towards a long wavelength in all samples. It can be noticed that the absorbance spectra in (Fig. 1) show different types of stones, as well as that each stone has different proportions of several components like whewellite, weddellite, uric acid, ammonium urate and carbonate apatite. Notice that sample 1 consists of 60% whewellite and 40% weddellite, while in sample 2 (70% whewellite, 20% ammonium urate, 10% carbonate apatite), sample 3 (80% whewellite, 10% uric acid dehydrate, 10% uric acid anhydrous), sample 4 (50% whewellite, 30% weddellite, 20% octacalcium phosphate pentahydrate), sample 5 (40% whewellite, 30% weddellite, 30% sodium urate), sample 6 (70% whewellite, 20% ammonium urate, 10% uric acid dehydrate), sample 7 (60% weddellite, 20% whewellite, 20% carbonate apatite), sample 8 (60% whewellite, 30% Struvite, 10% Brushite), sample 9 (87% whewellite, 10% protein, 3% carbonate apatite) and sample 10 (50% weddellite, 30% uric acid anhydrous, 20% carbonate apatite). It was found that the highest percentages of the components of the stones are calcium oxalate [9], so the kidney stone samples were classified as calcium oxalate, despite the presence of other components, but in relatively small proportions. It is noteworthy to acknowledge that the composition of renal calculi may exhibit variability across individuals. The makeup of a kidney stone may undergo alterations over a period of time. It is imperative to consult a medical professional for the analysis of kidney stones in order to ascertain their precise composition.

The optical absorption spectra depend on the chemical and crystal structure, thickness, and surface morphology of the stones (Fig. 2). show the optical absorption spectra of the calcium oxalate stones. The fundamental absorption was shifted towards a long wavelength. It can be noticed that the absorbance spectra in (Fig. 2) exhibited more significant absorption in the wavelength (0.0036–0.004 cm). At the same time, the absorbance was in calcium oxalate stones 57%. Sample 10 shows high absorbance due to a percentage of uric acid in its composition—the smallest absorbance in sample 7 is about (39%).

The absorption coefficient was calculated using (eq. (1)). The absorption coefficient as a function of photon energy is depicted in (Fig. 3). The absorption coefficient of all samples has a high value. From the figures, one can see the fundamental absorption coefficient, which was shifted towards the low energies

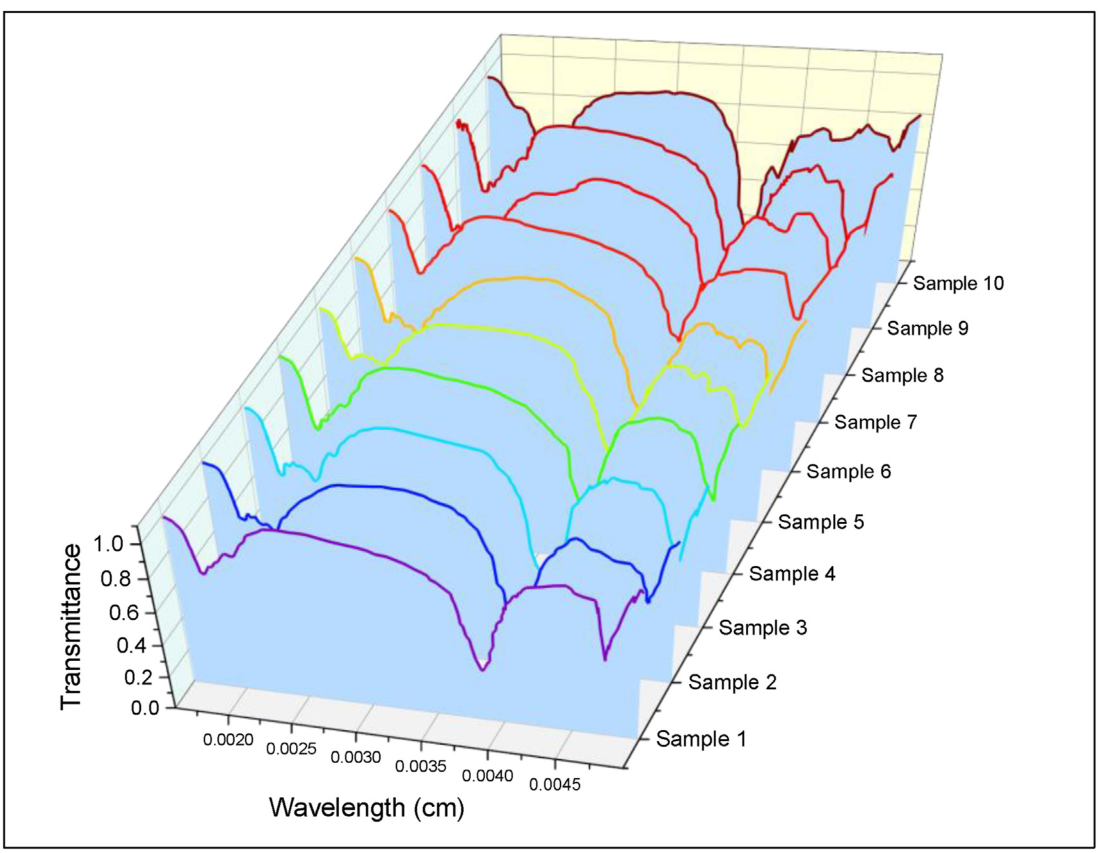

Fig. 4. Optical transmittance spectra of the calcium oxalate stone for samples.

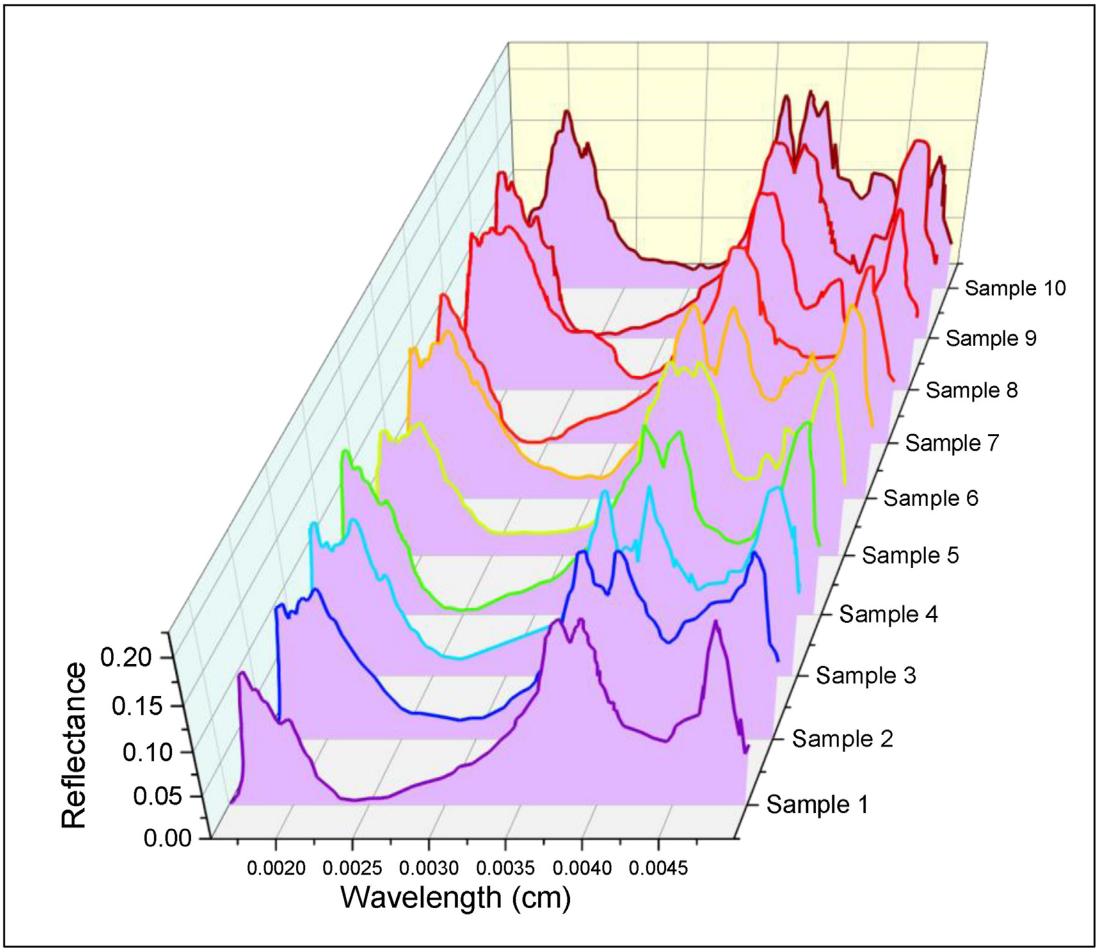

Fig. 5. Optical reflectance spectra of the calcium oxalate stone for samples.

(long wavelength), indicating that the stones absorb more light at lower energies is likely due to the presence of uric acid in the stones. Uric acid has a lower energy band gap than calcium oxalate, which means that it absorbs light at lower energies. The values of the absorption coefficient increase with the increase of uric acid content in calcium oxalate stones. The increase is also likely due to the presence of uric acid. Uric acid absorbs light more strongly than calcium oxalate, increasing the stones' overall absorption. The high absorption coefficient of calcium oxalate stones is likely due to the presence of calcium oxalate crystals. Calcium oxalate crystals are very small and have a high refractive index, which makes them good absorbers of light.

By using (eq. (3)), the optical transmittance was calculated. The optical transmittance spectra depend on the chemical structure, crystal structure, stone thickness, and the surface morphology of the stones (Fig. 4). shows the optical transmittance spectra of calcium oxalate stones. The transmittance spectra exhibit high transmittance values in the short wavelength beyond the absorption edge, decreasing in the wavelength range (0.0036−0.004 cm).

From (eq. (4)) calculate the reflectance with neglecting the scattering because it has the minimal value that can be neglected, and plotted as a function of wavelength in (Fig. 5) for calcium oxalate stones, the steep change of the reflectance in the absorption edge. It can be noticed that the highest optical reflectance peaks shifted towards the long wavelength, and it decreased in sample 6. This observation suggests that the stone demonstrates enhanced light scattering properties, wherein light experiences several scattering events within the stone. This light scattering effect is beneficial to absorb several photons. The enhanced light scattering may be attributed to surface morphologies or different compositions.

6. Conclusions

The results of this study suggest that the most common component of kidney stones is calcium oxalate. This is followed by ammonium urate, uric acid, and carbonate apatite. The presence of other components, such as octacalcium phosphate pentahydrate and sodium urate, is less common.

It is important to note that the composition of kidney stones can vary from person to person. The composition of a kidney stone can also change over time. This is why it is important to have kidney stones analyzed by a doctor to determine the exact composition.

The results of this study are consistent with previous studies that have shown that calcium oxalate is the most common component of kidney stones [5,6]. The presence of other components in kidney stones, such as ammonium urate, uric acid, and carbonate apatite, can vary depending on the individual's diet and risk factors for kidney stones the optical absorption spectra of calcium oxalate stones can be used to assess the chemical composition and structure of the stones. This information can be used to diagnose the type of stone and to develop treatment plans. The surface morphology of the stones can also affect the optical absorption spectra. The optical absorption spectra can be used to monitor the growth of calcium oxalate stones, and also can be used to develop new methods for treating calcium oxalate stones.

The absorption coefficient of all samples was high, indicating that calcium oxalate stones absorb light well. The fundamental absorption coefficient was shifted towards the low energies (long wavelength), These results show that calcium oxalate stones with a high uric acid content are more likely to absorb light than stones with a low uric acid content. This could be useful for developing new methods for detecting and treating kidney stones.

The optical transmittance spectra of calcium oxalate stones exhibit a high transmittance value in the short wavelength beyond the absorption edge. This indicates that the calcium oxalate stones have high transparency in the short wavelength region.

The reflectance of calcium oxalate stones decreases with increasing wavelength, and the highest optical reflectance peaks shift towards the long wavelength.

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