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Fourier Transform Infrared Spectrophotometer IRSpirit™-X

Application News

FTIR Analysis of Kidney Stone Using IRSpirit-TX

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User Benefits

- FTIR analysis of kidney stones can be easily performed with minimal sample preparation using QATR™-S.
- Quick identification of kidney stone composition is possible with LabSolutions™ IR software by searching the measured spectrum against the IR Kidney Stones Library.

■ Introduction

In the field of nephrology, FTIR analysis of kidney stones is a critical tool for studying nephrolithiasis etiology. The primary purpose of this analysis is to accurately identify the chemical composition of kidney stones, which can vary significantly among individuals. This information may provide insights into underlying metabolic disorders or dietary factors.

By employing FTIR spectroscopy, researchers can obtain detailed spectral data that enables the precise classification of stones, such as calcium oxalate, uric acid, struvite, or cystine [1]. This information can be beneficial for understanding the characteristics of kidney stones, potentially informing future research directions. Furthermore, FTIR analysis requires only a small volume of sample, allowing analysts to reserve more samples for other analytical techniques such as scanning electron microscopy, energy-dispersive X-ray spectroscopy, thermogravimetry and differential scanning calorimetry.

This Application News describes the simple workflow of kidney stone sample preparation and measurement by attenuated total reflection (ATR) method, followed by composition identification through a library search with the IR Kidney Stones Library.

Fig. 1 IRSpirit™-X with QATR™-S

■ NICODOM IR Kidney Stones Library

The NICODOM IR Kidney Stones Library is a collection of 1668 KBr pellet transmission spectra derived from different types of human kidney stones and related chemicals, including oxalates, phosphates, urates, other minerals and their mixtures, as well as stones of drug or organic origin. This library provides a basis for fast and reliable identification of kidney stone composition.

■ Sample Preparation

The conventional sample preparation method for kidney stone analysis is the KBr pellet technique. Although this technique can generate spectra with good sensitivity, the quality of the spectra can be affected by the potential moisture content in KBr and the homogeneity of the sample-KBr powder mixture. Therefore, in recent years, ATR has become the favored technique due to the minimal sample preparation involved.

For this experiment, several pieces of kidney stone samples were obtained from a medical center in the Philippines. One of the pieces was pulverized with an agate mortar and pestle as shown in Fig. 2.

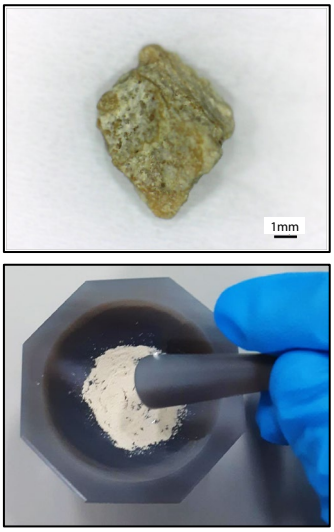

Fig. 2 Kidney Stone Sample Before (Top) and After (Bottom) Pulverization

■ Analysis Conditions

The pulverized sample was measured using IRSpirit-TX and QATR-S accessory (Fig. 1) with a zinc selenide (ZnSe) prism. A spatula of the powdered sample was pressed on the prism and measured under the analysis conditions specified in Table 1.

Table 1 Analysis Conditions

Instrument	: IRSpirit-TX and QATR-S (ZnSe)
Resolution	: 4 cm^{-1}
Accumulation	: 45 times
Wavenumber range	: 4000 – 500 cm^{-1}
Apodization Function	: SqrTriangle
Detector	: DLATGS

■ Compositional Analysis of Kidney Stone

ATR correction was performed on the acquired sample spectrum for better matching since the IR Kidney Stones Library is based on transmission spectra. Based on the search results as shown in Fig. 3, the sample spectrum closely resembles a mixture of carbonate apatite and struvite.

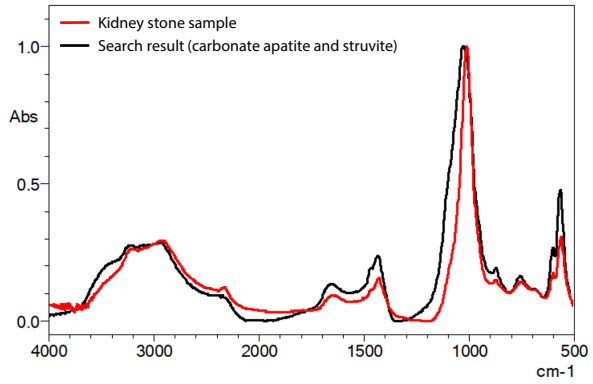

Fig. 3 Infrared Spectra of Kidney Stone Sample (Red) and Library Search Result (Black)

■ Conclusion

In this application news, the ATR technique using IRSpirit-TX is presented as a quick and easy solution for kidney stone characterization. This method provides valuable information that can enhance the understanding of the various factors associated with nephrolithiasis, potentially informing future research and studies in this area.

■ Acknowledgement

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<References>

1) M. Placzyńska, J. Milart, A. Lubas, J. Samotyjek, B. Jurkiewicz, B. Kalicki, K. Jobs. (2023) Association between the metabolic profile of urolithiasis in children with idiopathic hypercalciuria and the composition of the stone assessed by infrared spectroscopy, Pediatr Pol, 98 (4): 271-277

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IRSpirit-X series

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The IRSpirit-X series is a very compact infrared spectrophotometer that can be used with accessories from Shimadzu and other manufacturers.

It comes with IR Pilot™ software and provides 23 methods that can be used immediately without the need for parameter setting.

A comprehensive **10-year parts warranty** is provided with every purchase, giving you peace of mind for long-term reliable performance.

Three different models are available:

1) **Entry model IRSpirit-LX**
   Affordable option equipped with a lithium tantalate (LiTaO3) detector
2) **High-sensitivity model IRSpirit-TX**
   Equipped with DLATGS detector that can achieve high signal-to-noise ratio of 37,000:1, the highest among compact FTIRs
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QATR-S Single - Reflection ATR Accessory

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This is a horizontal ATR with a single reflection. A prism with a diameter of 1.8 mm is positioned horizontally, and the sample is pressed against the prism for measurement.

There are several options available for the prism material, each with their own unique benefits: diamond (high physical and chemical resistance), germanium (high refractive index) and zinc selenide (cost-effective option).

The clamp that holds the sample and prism in close contact has a built-in torque limiter which reduces the likelihood of damaging the prism by applying too much pressure.

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