



Application Note AN M131

Kidney Stone Analysis using ATR

Introduction

Most kidney stones contain calcium-phosphates, -oxalates, uric acid, or cystine as main components. Of course, mixtures of these substances are typical and the occurrence of many dozens of other materials is possible. Thus, only specialized analysis methods are capable to give reliable results. Fourier transform infrared spectroscopy (FT-IR) is one of the most powerful and cost-efficient methods for the analysis of kidney stones. It is very fast and does not require any chemicals or consumables like classical wet chemical methods. In contrast to X-ray diffraction IR allows to analyze amorphous substances.

The ATR-method presented in this application note has the benefit that there is no need for an extensive sample preparation, as it is the case with FT-IR spectrometers working in transmission or diffuse reflection. To perform the analysis the kidney stone sample simply has to be pressed on the ATR-measurement interface.

Keywords	Instruments and software
Urolithiasis	ALPHA Kidney Stone Analyzer
Medical treatment	OPUS spectroscopic software
Kidney stone analysis	Kidney stone wizard user interface
Infrared Spectroscopy	Spectral library of authentic kidney stones
Identification of components	
Attenuated Total Reflection (ATR)	

Method and instrumentation

The ALPHA Kidney Stone Analyzer is a dedicated system for the IR-spectroscopic analysis of kidney stones. It comprises the compact and robust ALPHA FT-IR spectrometer equipped with a diamond ATR (attenuated total reflection) measurement module (figure 1), a dedicated wizard software guiding through the analysis procedure and an extensive spectral library for the kidney stone identification. This library which contains more than 5000 spectra of authentic kidney stone samples was created and validated by Prof. Michel Daudon (Laboratoire Cristal, Hôpital Necker, Paris), who is a well-known expert for urolithiasis research.



Figure 1: ALPHA spectrometer with diamond ATR module

The ALPHA Kidney Stone Analyzer utilizes the ATR technique, as it provides a very convenient and fast way to measure all kinds of samples. Since the ATR-element is a pure diamond crystal brazed in the almost equally hard tungsten carbide, the measurement interface is extremely robust and durable and can handle even the hardest samples.



Figure 2: A kidney stone sample is being pressed on the diamond ATR crystal.

ATR measurements can be performed with very small sample amounts; a quantity of about 1 mg sample is sufficient for an analysis. Solid samples just need to be pressed on the ATR crystal via the one finger pressure applicator (see figure 2).

When the sample is in tight contact with the ATR crystal the IR radiation penetrates slightly (a few microns) into its surface and is reflected internally. The IR detector of the FT-IR spectrometer then can measure the wavelength dependent absorbance resulting from the sample.

With the aid of a specially designed software wizard, the user needs just one mouse click to start the measurement. After the measurement, the spectrum search is automatically performed and the result is displayed on the screen (figure 3). Altogether the measurement and search process takes just about a minute, which is much faster compared to the classical transmission method that needs at least ten minutes for the preparation of the sample-KBr pellet alone.

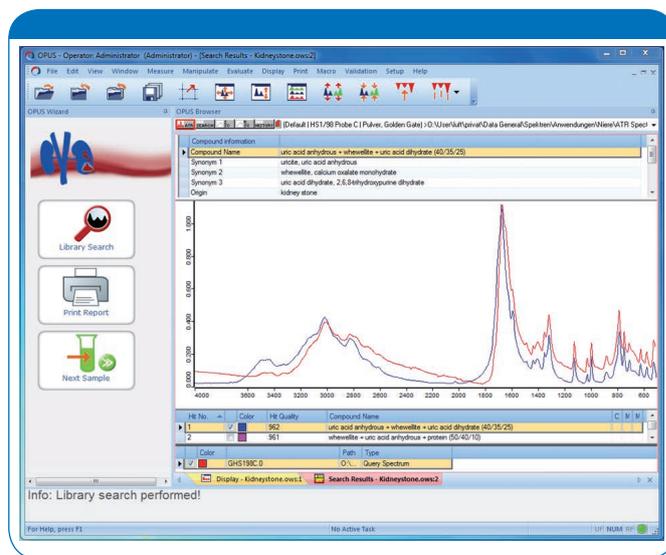


Figure 3: Software user interface of the ALPHA Kidney Stone Analyzer showing the identification result of an analyzed kidney stone.

As the ALPHA Kidney Stone Analyzer allows to perform an analysis quickly and without much effort it also facilitates multiple analyses of different fractions from the same stone. Due to the typically quite inhomogeneous structure of kidney stones this option helps to obtain a more detailed picture e.g. about the composition of the core and outer layers than just analyzing the homogenized stone.

Application example: Identification of kidney stone samples

After the measurement of a sample, the software automatically performs a spectrum search. During this process, the measured spectrum is automatically compared against a database of reference spectra. The similarity between the query spectrum and the database spectra is expressed in so called hit quality points. The higher the similarity the more hit quality points the database spectrum will get whereas the maximum number is 1000 points.

In the following figures the search results of different kidney stone samples are shown. Figure 4 shows the analysis of a stone with cystine as the main component with an excellent hit quality of 941 points. Additionally, the substance "carbonate apatite" was detected as a second component. The apatite content, however, seems to be considerably smaller than 5% since pure cystine is listed on the second position of the hit list with an almost equal hit quality of 940. The upper area of the result screen shows additional information about the selected library entry, like synonyms of the compound names.

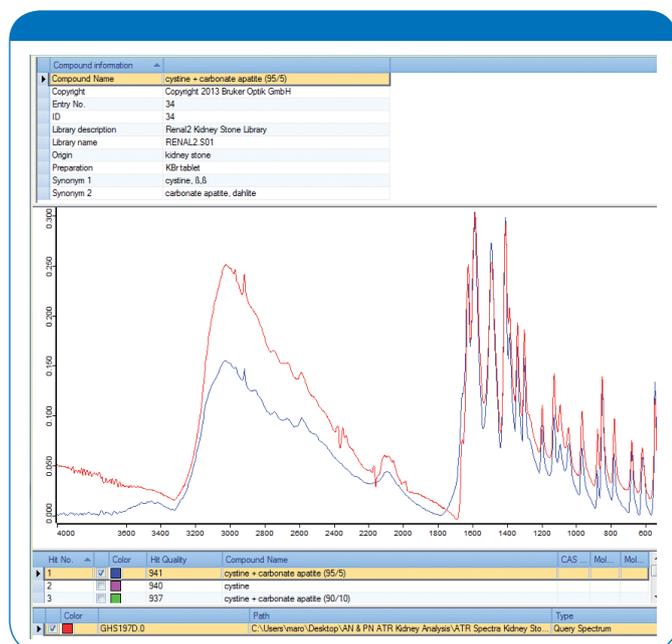


Figure 4: Search result of a kidney stone sample measured with the ALPHA Kidney Stone Analyzer. The main component of the kidney stone is clearly identified as cystine.

Figure 5 shows the search result of a second sample. Again, the first hit shows an excellent hit quality of 962 points and identifies the sample as a mixture of whewellite (calcium oxalate) and uric acid. Since the second hit has an almost equal hit quality of 961, the presence protein traces can also not be ruled out.

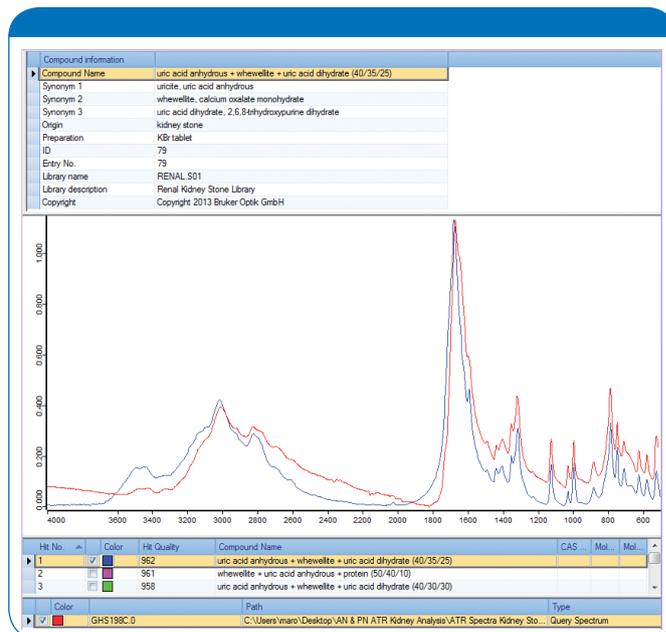


Figure 5: Search result of a kidney stone sample. The kidney stone contains a mixture of uric acid and whewellite.

Summary

The ALPHA Kidney Stone Analyzer is a robust and compact system with a diamond-ATR measurement interface and an extensive spectral library of real kidney stones. The ATR method allows a much faster analysis when compared to the classical transmission method, resulting in a higher sample throughput and a much more convenient measurement procedure. With the aid of the dedicated wizard and the included spectral library the identification of kidney stones can be performed in a very comfortable manner in just about one minute.

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