

## Application Note AN # 83

# Kidney stone analysis made simple

### Introduction

The incidence of urolithiasis in the general population is about 6-10 % and rises in various parts of the world. It is one of the most painful disorders that afflicts humans. Medical treatment includes removal of the kidney stone and the prevention of recurrent stone formation. An effective prevention is specific to the cause of stone formation, which can be determined from the chemical composition of the stone. As kidney stones often are built in layers around a seed crystal with different chemical composition, sampling of different parts of the stone is very important for the analytical result. About 85 different compounds have been detected in kidney stones, however, most of them occurring rarely. In more than 90 % of all cases various calcium oxalates and phosphates, ammonium magnesium phosphate, uric acid, or cystine are the main components.

Analysis of kidney stones with wet chemical methods is time consuming, not very reliable and requires a relatively large sample amount. Better results are obtained by using instrumental analysis methods (infrared spectroscopy, polarization microscopy, X-ray diffraction, UV/VIS spectroscopy). Of these, infrared spectroscopy is the most commonly applied technique, well suited for the qualitative and quantitative analysis of kidney stones. It allows to ana-

lyze both mineral and organic compounds and to distinguish between various crystalline phases of a certain compound. In contrast to X-ray diffraction, amorphous as well as crystalline compounds can be identified. Furthermore, infrared spectroscopy is cost effective, simple to use, very fast and requires only small sample quantities. Bruker offers two different approaches for the chemical analysis of kidney stones. Both are based on the ALPHA FT-IR spectrometer in combination with the following libraries:

- The BLG-1 library includes on diffuse reflectance spectra of ca. 500 synthetic mixtures of typical kidney stone compositions.
- And the BLG-2 library which contains transmission spectra of ca. 5000 authentic kidney stones.

Both libraries can in practice be used in combination with the ALPHA transmission unit and the ALPHA diffuse reflectance unit (DRIFT). Best results will of course be obtained when the sample spectra are measured with the same measurement technique as the library spectra. In order to simplify the measurement and evaluation, the OPUS software provides an additional "Wizard"-interface. The Wizard allows even untrained users to measure and evaluate kidney stone samples within just a few minutes.

## Instrumentation

The very compact ALPHA FT-IR spectrometer is a robust and affordable system that is very easy to operate. It produces reliable and reproducible data. A permanent online diagnostics of the spectrometer by the Performance-Guard™ provides a “real time” display of the instrument status. Instrument validation (OQ/PQ) is performed by fully automated test routines to ensure permanent instrument operation within specification.

Besides the ALPHA is a very versatile system. The ALPHA QuickSnap™ mechanism allows the exchange of sampling modules within just a few seconds and without the use of any tools. Newly installed modules like a transmission, DRIFT or an ATR unit are recognized instantly by the ALPHA spectrometer. After an automatic performance test the optimal set of measurement parameters is loaded.

The measurement process itself is very comfortable by means of a specially designed Wizard. Even untrained users are able to measure and evaluate a sample in less than a minute. During the measurement and evaluation process the Wizard changes its appearance dynamically, by doing so the user is guided step by step through the whole analytical process. As an example figure 2 shows the appearance of the user interface after two measure-



Figure 1: ALPHA FT-IR spectrometer with diffuse reflectance unit (DRIFT) and transmission module (upper left corner). The inset also illustrates the simple sampling module exchange via QuickSnap™.

ments have been completed and analyzed. The Wizard, located on the left side of the OPUS window, now offers the possibility to measure a new background or to proceed with the measurement of a new sample.

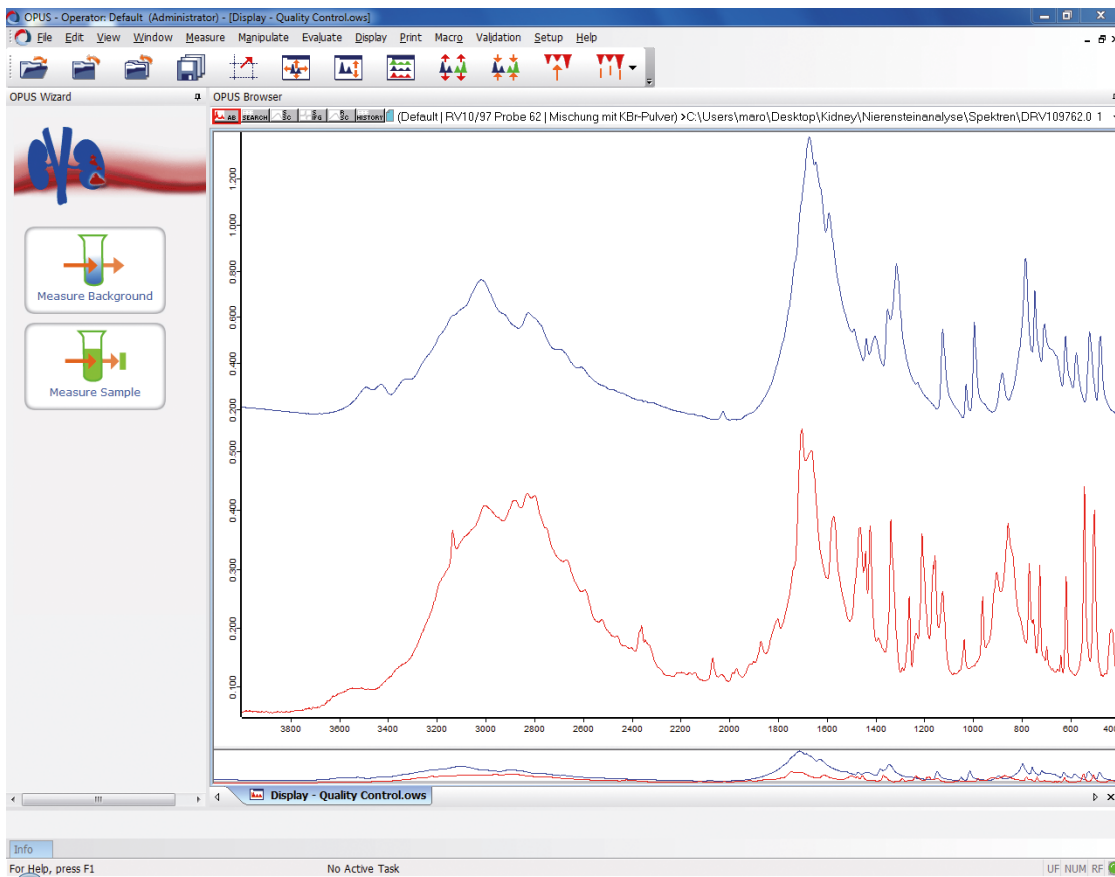


Figure 2: OPUS user interface with the Wizard bar on the left. The spectra display shows two typical kidney stone spectra.

## Procedure Measurement

The measurement and analysis of kidney stones using FT-IR is very fast and easy. The kidney stone is broken and ground. 1-3mg of the powder is mixed with potassium bromide (ca. 100 mg - 300 mg). This mixed powder can be directly used for a DRIFT-measurement or has to be compressed into a pellet in order to use it for a transmission measurement.

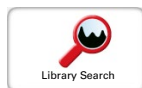
- To measure the background press the “Measure Background” button of the Wizard:



- Place your sample in the sample holder and close the sample compartment.
- Measure the spectrum by a click on the “Measure Sample”-button:



After the measurement you will see the following buttons on your Wizard bar:



To identify the kidney stone sample you can perform a library search by simply pressing the “Library Search”-button. The “Print Report”-button allows you to print your sample spectrum or your library search result with just one mouse click. A click on the “Next Sample”-button will close the search result and the Wizard will offer you to measure a new sample or to measure a new background first.

The result of the library search will appear in form of a list showing the most probable hits together with a hit quality number that has a value up to 1000 depending on the correlation of both sample and library spectrum. Each hit entry includes the chemical composition of the corresponding kidney stone. Moreover, the weight ratio of up to three dominating components is suggested. An example result is displayed in figure 3; the measured spectrum is displayed together with the best hit in the middle of the result window.

You can also display other spectra from the result list by simply clicking on the checkboxes on the left of the search results. On top additional information on the library entry is listed.

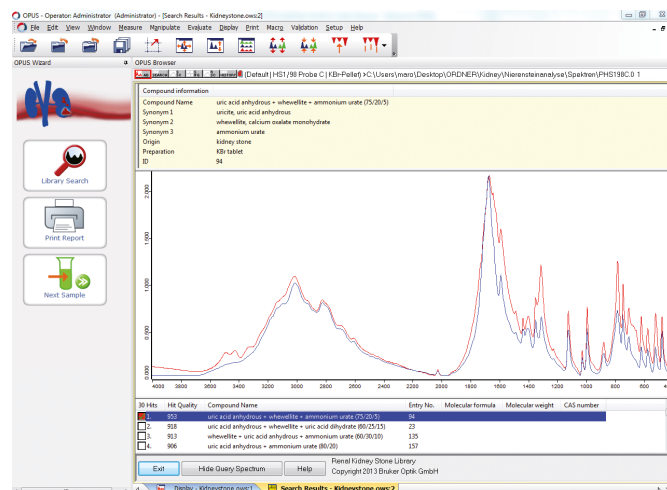


Figure 3: Result of a spectrum search with the hitlist and the sample spectrum displayed together with the library spectrum.

## Summary

The combination of the compact and robust FT-IR spectrometer ALPHA with a dedicated software wizard and comprehensive spectra libraries results in a reliable and user friendly analysis system for kidney stones.

Spectra search in the provided libraries accomplishes the identification of the kidney stones' major components together with an indication of their quantitative ratio. Due to the easy handling of the ALPHA instrument and wizard guided measurement, evaluation and reporting can be performed even by untrained users.