

HANDHELD FTIR ANALYZERS

A NEW CAPABILITY FOR AT SITE MEASUREMENTS OF ROCK AND MINERALS - DIFFUSE REFLECTANCE GEOLIBRARY



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INTRODUCTION:

Just recently, A2 Technologies announced the availability of the first handheld battery operated FTIR analyzers that have both the performance envelope and robustness to be used effectively in demanding field environments. A particularly useful application for this technology is in the geosciences and in this application brief, we will discuss the use of A2 Technologies Exoscan and FlexScan systems [figure 1] in the development of a rock and mineral library optimized for a field FTIR analyzer.

FTIR spectroscopy has been used for years in the study of rocks and minerals and there are a number of commercially available libraries containing geological samples. These libraries all have the common trait of being measured in classical absorbance/transmittance mode. This typically entails taking a small specimen of mineral and grinding it in KBr or nujol to make a suspension to record the spectrum of the mineral. The other common trait is that all of these spectra were recorded in a lab using a traditional bench top FTIR spectrometer.

The complement to an at-site IR analyzer is the ability to record a spectrum with little or no sample preparation. This allows the IR spectrum of an area of interest to be obtained, whether it is in an outcrop, ore body, drill core, or inside a mine. For this reason, we have developed a diffuse reflectance sampling interface for our handheld FTIR systems, which enables direct measurement of samples without sample preparation.

This form of reflectance measurements collects the diffusely scattered light from a sample and then returns the scattered light to the IR detector. Diffuse reflectance of neat rocks and minerals differ from transmittance spectra and thus we are creating a unique library for this type of analysis method that is contained on-board the analyzer. Igneous/plutonic, metamorphic and sedimentary rocks and minerals are included in the library possessing various chemical compositions including nitrates,



Figure 1 - A2 FTIR analyzer with diffuse reflectance sampling interface rapidly records the molecular spectrum of the sample with no preparation required.

sulfates, oxides, silicates, aluminosilicates, phosphates, sulfides, borates, vanadates, tungstates, uranates etc. If a mineral possesses a chemical structure in which the atoms are covalently bonded, there is frequently a well defined infrared spectrum that is obtained.

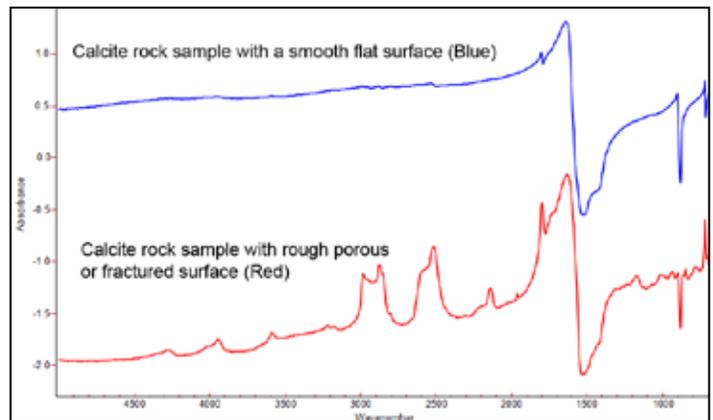


Figure 2 - Stacked plot of spectra of calcite rock samples with a smooth flat surface (Blue) and a rough porous or fractured surface texture (Red) from representative mineral chemical composition classes. The spectra were recorded at 4 cm⁻¹ resolution and consist of 128 scans coadded interferograms that take approximately 1 minute to collect and process

Depending on the particle size and crystallinity of the specimen, as well as the reflectivity of the surface being analyzed, there can be a specular component to the diffuse reflectance spectrum, which tends to alter the overall spectrum. Therefore, for certain minerals, we have included spectra in the library of both the rough surface and the smooth reflective crystal surfaces [figure 2]. The algorithm used by the analyzer accesses both types of spectra to predict the best match for a particular sample.

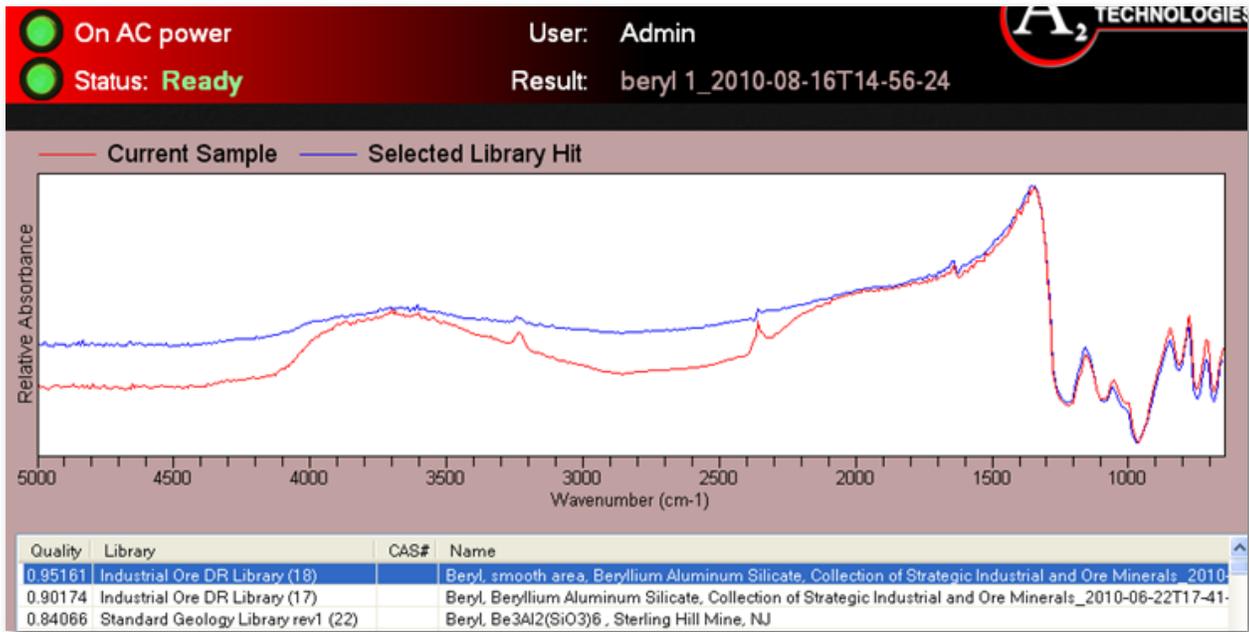


Figure 3 - The infrared spectrum of minerals measured neat may arise from diffuse and specular reflection and thus both types of spectra are included in the library, thereby maximizing the potential hit quality

The intuitive software of the A2 FTIR analyzers enables the user to quickly ascertain the identity of a mineral in the field [figure 3]. The full spectrum of the specimen in question is stored and can be accessed for further investigation. As more referee specimens become available, we will continue to expand the diffuse reflectance rock and mineral library. In addition to the on-board A2 library, the Exoscan and FlexScan FTIR analyzers allow users to easily create their own library specific to their requirements



The availability of a field ready FTIR analyzer that provides molecular composition analysis of rocks and minerals with little or no sample preparation, coupled with an on-board library to assist in identification, is a powerful new tool for the geoscientist, and an important complement to elemental analysis analyzers that are already in use in the field.

