



Application Note AN #88

Teaching FT-IR-spectroscopy with the ALPHA

With the footprint of a lab book, the FT-IR spectrometer ALPHA is a perfect fit for classrooms and teaching laboratories: It combines a high performance optic delivering excellent sensitivity, measurement stability and x-axis accuracy at an affordable price. Due to its small size, the ALPHA can be placed almost everywhere. Being robust and generating reliable high quality data the ALPHA is suitable for educational and research applications alike. The ALPHA's smart hard- and software design makes FT-IR analysis simpler than it has ever been before.

As an ideal addition for teaching, Bruker offers a comprehensive teaching kit (fig. 2) which includes a starter package, a dedicated wizard guided user interface and a detailed instruction manual explaining several standard experiments in education. The starter package contains a liquid cell for Lambert-Beer based quantification measurements, a magnetic foil holder together with the extensive Bruker polymer library for the identification and thickness determination of polymer foils and a gas cell with an additional aperture. With the aid of the teaching wizard and the manual, an IR training course can be prepared easily and the students will be able to measure and evaluate their samples without the need of an extensive introduction



Instrumentation

The ALPHA is a very compact and robust spectrometer and therefore ideally suited for educational purposes. It is equipped with wear free components like the patented RockSolid interferometer and a durable solid-state diode laser. The infrared source and the desiccant are user replaceable; there is no need for an external service since both consumables are easily accessible through the back of the instrument.

Long life components, extremely user-friendly maintenance and the ALPHA's low energy consumption result in incomparably small running costs. Due to the unique design, the ALPHA is rugged and insensitive to external disturbances like e.g. impacts and vibrations. Therefore, the instrument can be moved safely and, with a weight of only 7 kg and its compact dimensions, also very easily.

The ALPHA is a highly flexible instrument since Bruker offers a wide range of accessories like for instance various transmission, attenuated total reflection (ATR) and diffuse and specular reflectance units that can be exchanged without the use of any tools.



Figure 1: ALPHA accessories with QuickSnap™ accessory exchange.

Application Examples

Example 1: The vapor phase spectrum of the heteronuclear diatomic molecule hydrogen chloride (HCl) is an ideal example to illustrate the principles of ro-vibrational spectroscopy and therefore a classical experiment of physical chemistry. In order to show the rotational fine structure a highly resolving FT-IR spectrometer is needed. With the high-resolution option for the ALPHA, excellent spectra of HCl vapor can be obtained. Figure 4 shows the ro-vibrational spectrum of HCl measured with the depicted gas-cell. The fine structure is clearly resolved and the magnification in figure 5 displays the split of the rotational bands resulting from the natural chlorine isotopes ^{35}Cl and ^{37}Cl . All necessary parts for this experiment are assembled in the teaching kit, notably the gas cell which is built from the corrosive

resistant V4A (1.4401) steel and fitted with CaF_2 -windows that are resistant against water and HCl gas. With this cell, it is possible to retrieve the HCl gas very conveniently from the headspace of fuming hydrochloric acid.



Figure 2: Constituent parts of the teaching kit in front of an ALPHA: Liquid cell, magnetic foil holder and gas cell with aperture. The display of the laptop is showing the wizard with a measured gas spectrum.

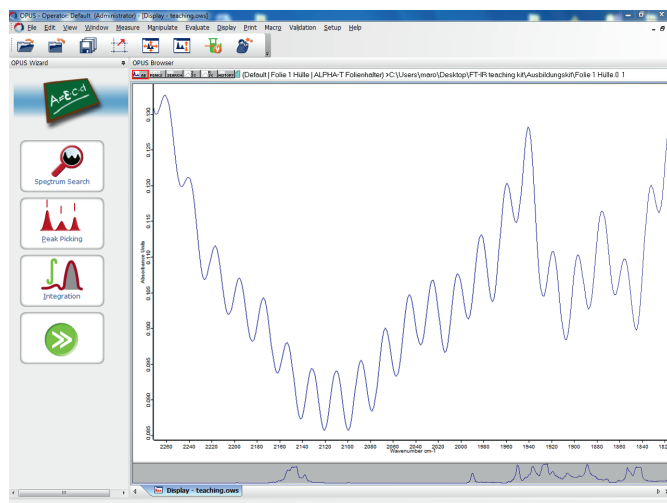


Figure 3: View of the teaching wizard with fringes of a polymer foil.

The teaching kit contains further fully elaborated experiments: Besides a detailed Lambert-Beer based quantification experiment of cyclohexanone in cyclohexane the students are learning how to identify a polymeric foil via a library search and subsequently determine its thickness by the analysis of the interference fringes. The dedicated wizard in combination with the manual guides the students through the experiments, provides background information and minimizes the preparation time for the teacher and the students alike.

Example 2: The handling and analysis of air and moisture sensitive samples is an important task for research projects

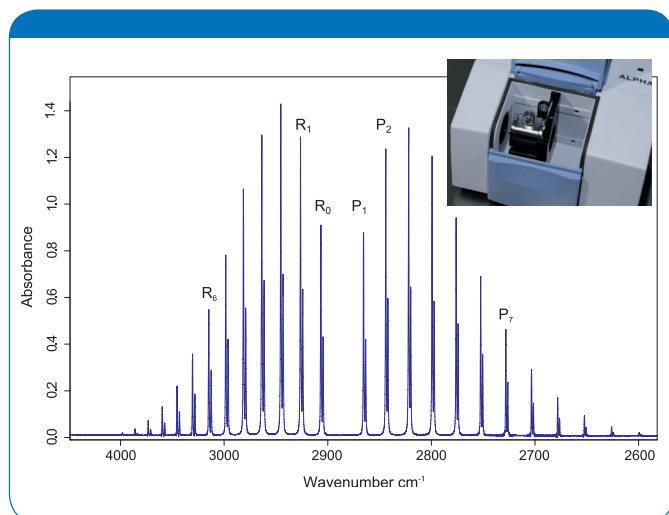


Figure 4: The ro-vibrational vapor phase spectrum of HCl measured with the ALPHA in transmission

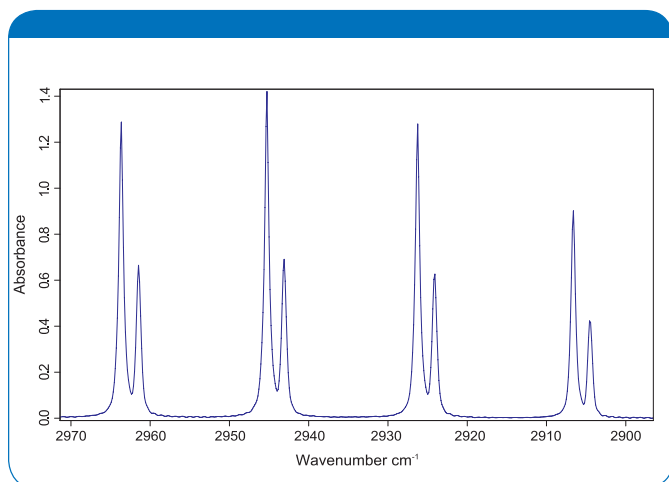


Figure 5: Zoom of the spectrum; the ro-vibrational lines are split due to the chlorine 35 and chlorine 37 natural isotopic ratio

as well as for the education of chemists and laboratory assistants. The ALPHA spectrometer can be placed easily inside every standard glovebox and is, in combination with the Platinum diamond ATR unit, the most elegant way to measure sensitive samples (see figure 6). The ALPHA is stable in a vacuum environment and can be transferred easily through the antechamber of the glovebox. The internal desiccant can be removed by the user, ensuring rapid exchange of the air inside the spectrometer with the inert gas atmosphere. The ALPHA can even communicate with a computer outside the glovebox via a wireless connection. With the aid of the one finger clamping mechanism, the samples can be easily placed into position for analysis, even when wearing thick rubber gloves. Clearly, using an FT-IR spectrometer inside the glovebox is safer, easier and much faster than transferring the samples out of the glovebox.

Example 3: In chemistry lab courses, the compounds synthesized by the students need to be analyzed to verify their



Figure 6: ALPHA spectrometer inside a glovebox.

identity. By using an ALPHA in combination with an ATR module, the whole task of sample measurement, evaluation and report generation can be accomplished in less than a minute. After measurement of the compound, its spectrum is compared against selected spectra libraries. The library search will result in a hit list with the most probable substance on the top. The higher the “Hit Quality” (max. 1000), the better the correlation between the sample spectrum and the library spectrum. Our example in figure 7 shows the result of a library search on synthesized acetylsalicylic acid. With a hit-quality of 940, the substance is clearly identified. Additional information such as the molecular formula and the chemical structure is shown on top of the search result window. Bruker offers a wide variety of spectra libraries containing thousands of organic and inorganic substances. For specific classes of compounds like pharmacological substances or polymers dedicated libraries are available.

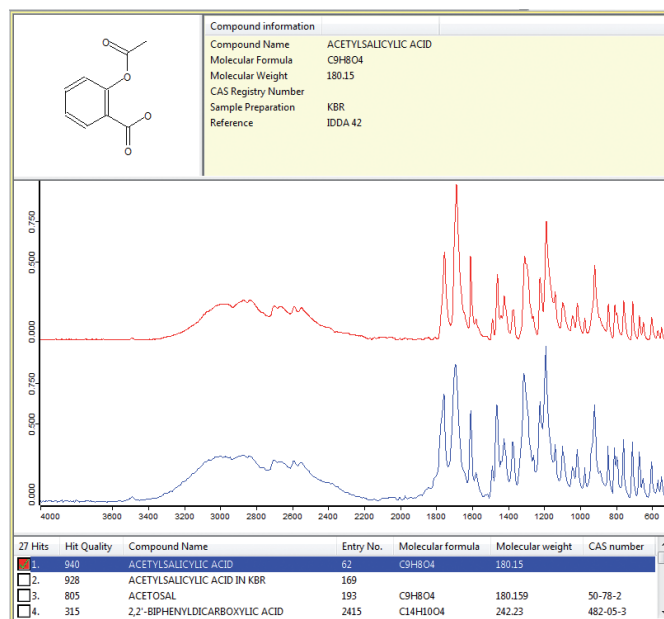


Figure 7: Search result window with hit list entries.

Summary

The Bruker ALPHA spectrometer offers a wide range of possible applications in the field of education and academia. It is very flexible with many different accessories. The Bruker Platinum diamond ATR for example, allows easy and fast sample measurement, even with thick rubber gloves inside a glovebox. Thanks to the QuickSnap™ mechanism, any accessory can be attached very quickly, instantly supplying an integrated spectrometer system for the next measurement task.

The additionally available teaching kit is an ideal tool to impart knowledge about FT-IR spectroscopy to the students. The starter package contains all necessary parts for the measurement of liquids, foils and gases. The instruction manual highlights both the practical and theoretical background of the subjects taught. Combined with the dedicated software wizard the manual provides perfect guidance of the students through all the experiments without the need to acquire specific skills on the spectroscopic OPUS software.

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