Product Note M31-10/11

A173/B
PMA 50 Polarization Modulation Accessory PMA 50

The PMA 50 is an accessory to be used in conjunction with any Bruker Optics VERTEX and TENSOR series FT-IR spectrometer. By modulating the polarization of the infrared light, it can be used for several different experiments, such as to investigate chiral molecules or to probe trace quantities of surface-sorbed species. It consists of a housing with input for a modulated IR beam, a photoelastic modulator (PEM), a specialized sample holder (depending on the experiment), along with non-polarizing focusing optics and detector. The filter and demodulation electronics are an integral part of the system and special software has been developed for processing polarized data.

The PMA 50 is modular in design and is attached to the side of the spectrometer, keeping the FT-IR sample compartment free for other applications.

All components of the PMA 50 have been optimized in their design to provide outstanding results in polarized spectroscopy.

Applications

1) VCD: Optically active species, e.g. chiral molecules, exhibit Circular Dichroism (CD). This is a non-zero differential absorption of left- or right-circularly polarized light. If one is monitoring vibrational transitions in the infrared region, the phenomenon is referred to as Vibrational Circular Dichroism (VCD). High sensitivity is required for VCD measurements due to the small absorption differences, typically between 10^{-4} and 10^{-5} absorbance units. This is achieved by applying the polarization modulation (PM) technique using a photoelastic modulator (PEM). Using these PM techniques VCD spectroscopy has become a powerful tool for the analyst to obtain structural information at the molecular level. The optical purity of enantiomers and (in combination with ab initio

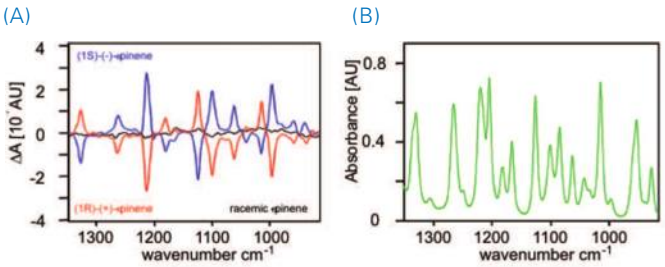

Fig. 1: VCD (A) and absorption (B) spectra of (1R)-(+)-pinene (red) and(1S)-(-)-a-pinene (blue). Spectra were collected as the neat liquid in a 50µm KBr cell with a resolution of $4cm^{-1}$.

calculations) the absolute configuration of chiral molecules can be determined with a high degree of accuracy. Another important field of application is the conformational analysis of biomolecules (e.g. the secondary structure of proteins or DNA), which makes VCD an attractive analytical method for organic and biological chemistry as well as for the pharmaceutical industry.

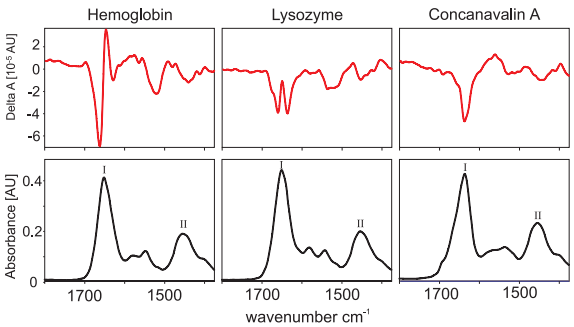

Fig. 2: Absorption (bottom) and VCD spectra (top) of hemoglobin, lysozyme and concanavalin A in D_2O solution

2) PM-IRRAS: Infrared reflection-absorption spectroscopy (IRRAS) is a well established technique for studying substances adsorbed on metal surfaces. As the name suggests the infrared light is reflected off a metallic surface rather than transmitted through the sample as in the VCD configuration. The technique in general can be extended by applying polarization modulation (PM) technique to the IRRAS experiment. It takes advantage of the difference in the absorption of p- and s-polarized light at high angles of incidence. In particular, using PM methods the sensitivity

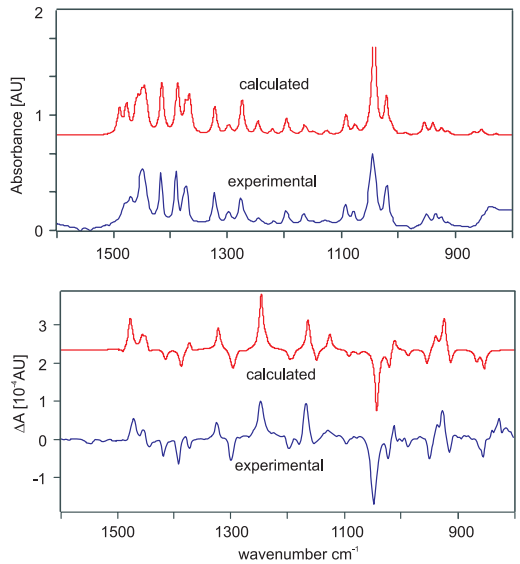

Fig. 3: Top: absorbance spectra of (+)-camphor, calculated (red) and measured (blue). Bottom: VCD spectra of (+)-camphor, calculated (red) and measured (blue).

can be significantly increased thus facilitating the investigation of very thin films, such as molecules adsorbed from the gaseous phase, or organic monolayers deposited onto a metal surface.

Standard system components and features

- Filter holder for selecting desired optical filter
- Rotatable linear polarizer in front of the photo-elastic modulator (PEM)
- PEM: ZnSe, 42 kHz, AR-coated
- Sample holder for VCD and VLD measurements, variable optical path length
- PM-IRRAS sample holder with continuously variable rotation stage and self-masking sample mount; sample reflecting surface remains at focal point. Reflection measurements are between 70° and 89° with angle scribe marks
- Non-polarizing beam focussing with a lens
- MCT-Detector with non-dichroic BaF_2 window
- Specially adapted electronics integrated into the PMA 50 module, easy operation
- Dual channel acquisition for both signals
- Specially designed software for data calculation
- Full-integrated demodulation electronics for compact design and easy operation
- Continuously variable resolution
- Broad spectral range depending on configuration. Base configuration 4000 - 750cm^{-1}