INFRARED SPECTROMETER ACCESSORIES

Extended Range with the KRS-5 Focusing Lenses

Introduction

To operate successfully, micro-ATR accessories use a combination of optical components to direct and focus the infrared beam onto the ATR element. For diamond ATR's, one of the most critical is the focusing element. ZnSe tends to be the material of choice because of its high throughput and physical properties allowing data collection to as low as 650 cm-1. The use of the optional KRS-5 focusing lenses extends the working range, providing additional data down to 250cm-1 (350 cm-1 with a KBr beamsplitter).

This paper discusses the additional data obtained while using the KRS-5 focusing lenses with the Golden Gate™ diamond micro-ATR.

Specac's Golden Gate ATR Accessory

Virtually any solid or liquid sample can be examined with the Golden Gate™ micro-ATR accessory. Solids, liquids, single crystals, fibers, pastes, gels and aqueous solutions can all be examined with little or no sample preparation.

Compared to traditional infrared analysis methods, the micro-ATR accessory provides one of the most universal sampling methods for the collection of infrared spectra. While the mid-infrared range is generally considered to be 4000 - 400 cm-1, the loss of a few hundred cm-1 at the low end of the spectrum is an accepted sacrifice for the convenience and utility of the ATR method.

But spectral analysis using the Golden Gate ☐ ER (Extended Range) provides a more complete picture of the mid-infrared spectrum. The spectral range limitation for a traditional diamond micro-ATR accessory is eliminated when using the optional KRS-5 focusing lenses in the Golden Gate™. Spectral detail that may be essential for positive sample identification or specific vibrational studies can be obtained with all of the ease and flexibility of the standard

Golden Gate™ micro-ATR. By simply replacing the ZnSe focusing lenses with the optional KRS-5 lenses, spectral data can be obtained throughout the standard mid-infrared region and well into the far-infrared (useful range 4000-250 cm-1).

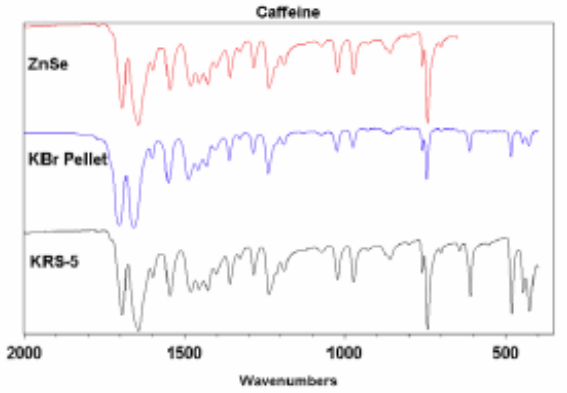

Figure 1

Experiment and Results

All spectra were collected using a Golden Gate™ micro-ATR accessory equipped with a single-reflection diamond ATR element. Initially, the ZnSe lenses supplied were used to collect a range of sample spectra, then the optional KRS-5 lenses were installed and additional spectra collected from the samples. No sample preparation was necessary to obtain the various spectra and the samples were simply cleaned from the crystal surface after data collection.

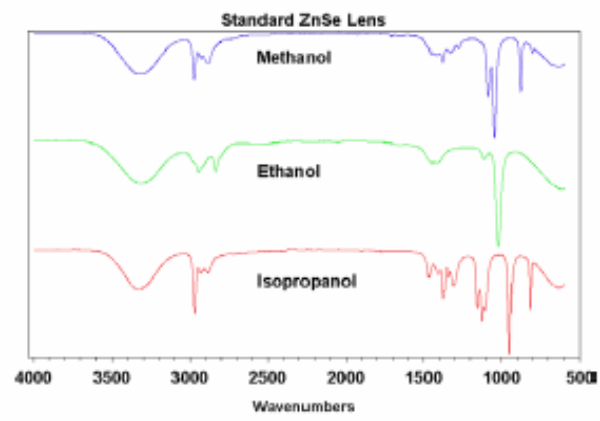

Figure 2

FT-IR spectra of 64 scans at 4 cm-1 resolution were coadded and averaged to obtain all single-beam background and sample spectra.

Figure 1 illustrates the fingerprint region (2000 - 400 cm-1) of the transmission and ATR spectra of caffeine. The ZnSe and the KRS-5 lenses were used to collect the ATR spectra and are plotted with a KBr pellet spectrum of caffeine. Note the enhancement of the lower wavelength vibrations for the ATR spectra as compared to the KBr pellet spectrum.1 The additional data provided by the KRS-5 version of the Golden Gate™ exactly matches the wavelength values for the transmission sample peaks within 0.75 cm-1.

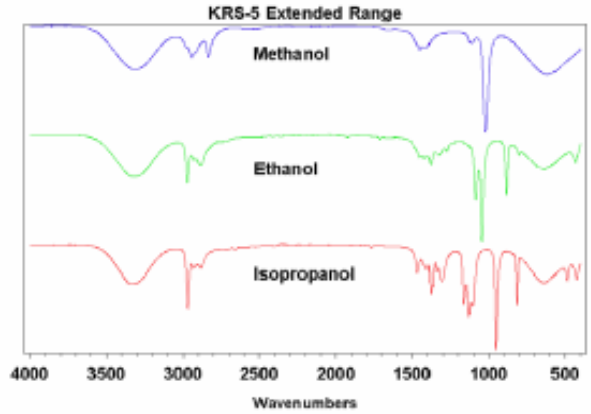

Figure 3

Figures 2 and 3 are plots of methanol, ethanol and isopropanol using the ZnSe and KRS-5 lenses, respectively, in the Golden Gate™ micro-ATR. The

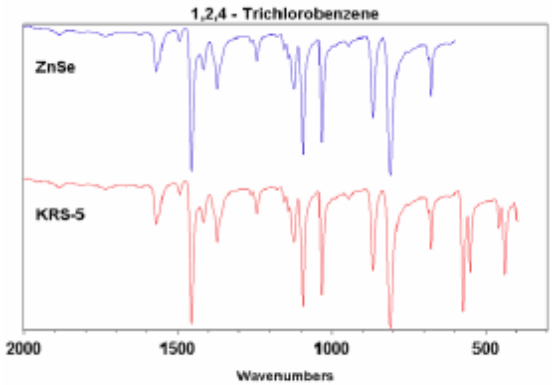

Figure 4

KRS-5 lens enables analysis of the C-O-H out-of-plane bend and the skeletal deformation modes, which are not visible in the ZnSe spectra.

Figure 4 is a plot of 1, 2, 4 - trichlorobenzene using the ZnSe and KRS-5 lenses. The additional spectral range provides data corresponding to the C-Cl and ring bending modes.

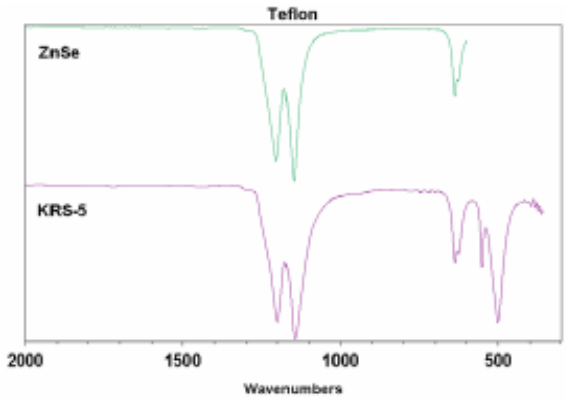

Figure 5

Of particular interest is the spectra collected for a sample of poly(tetrafluoroethylene) (PTFE). The KRS-5 lens provides much more detailed spectral information critical for positive identification. Certainly, the search of a standard ATR spectral library would recognize the ZnSe spectrum, but the KRS-5 spectrum reveals the additional C-F bending modes and makes the characterization routine.

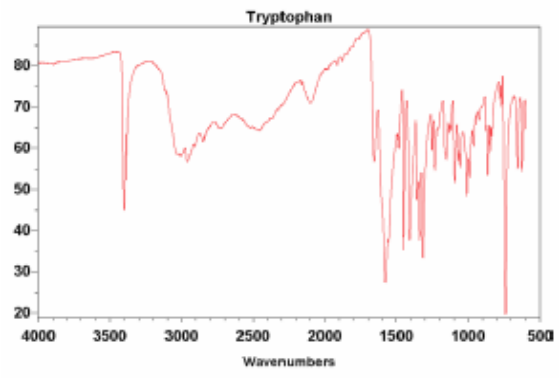

Figure 6

Figure 6 is a plot of the ZnSe spectrum of tryptophan, with the rich detail of the fingerprint region illustrated as Figure 7. Again, the ZnSe spectrum is recognizable from other amino acid spectra, but the additional spectral range provided by the KRS-5 lenses offers additional vibrational data.

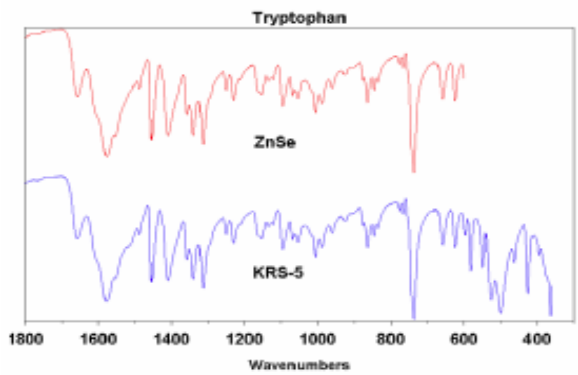

Figure 7

Conclusion

The Golden Gate™ single reflection micro-ATR is a simple, easy-to-use accessory for the analysis of solids, liquids and solutions. The use of the optional KRS-5 focusing lens for the Golden Gate™ accessory enhances the simple, rapid and very reliable ATR technique. The analysis method is non-destructive and can be used to collect data from a minimal amount of sample.

References

1. Gilby, A. C., Cassels, J., and Wilks, P. A., Applied Spectroscopy, 23(5), 1970.

Acknowledgements

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