INFRARED SPECTROMETER ACCESSORIES

Analysis of Drugs of Abuse

- Non destructive sample analysis
- No sample cross contamination
- Reproducible results
- Searchable spectral libraries
- No sample preparation

The above represent some of the key criteria for today's modern forensic scientist.

Introduction

An important application of Fourier Transform infrared (FT-IR) spectroscopy is the forensic analysis of drugs of abuse.

Whether controlled narcotics or illegally obtained 'street' drugs, samples are routinely submitted for chemical analysis.

In today's fast paced investigative world where case numbers are escalating to almost unmanageable levels and data is subject to extreme cross examination, it has become very important to use methods of analysis that eliminate the risk of user error, are quick and easy to use, are reproducible and eliminate the risk of sample cross contamination. They also have to be non-destructive allowing the sample to be either presented as evidence or available for further analysis.

The traditional method of analysis for powders and tablets is to grind them up with Potassium Bromide (KBr), press into a pellet or disc and collect an infrared transmittance spectrum.

Specac's Golden Gate ATR Accessory.

Making a 'good' KBr pellet takes practice and the quality of the spectra is often questionable and difficult to re-produce. The original sample cannot be recovered for presentation as evidence or further analysis.

The Golden Gate™ Diamond Attenuated Total Reflectance Accessory provides a solution to all these problems.

The neat powder or solid sample is placed onto the diamond ATR crystal, clamping pressure is

applied, and the sample spectrum is collected. The crystal surface is wiped clean and the accessory is ready to collect additional spectra.

The procedure is less complicated and much faster than the KBr pellet technique and subject to fewer potential user errors.

Caution must be observed, however, when attempting to directly compare ATR and transmission spectra. Changes in the relative peak intensity of the absorption bands, does occur, and is a result of the internal reflection mechanism of ATR accessories[1].

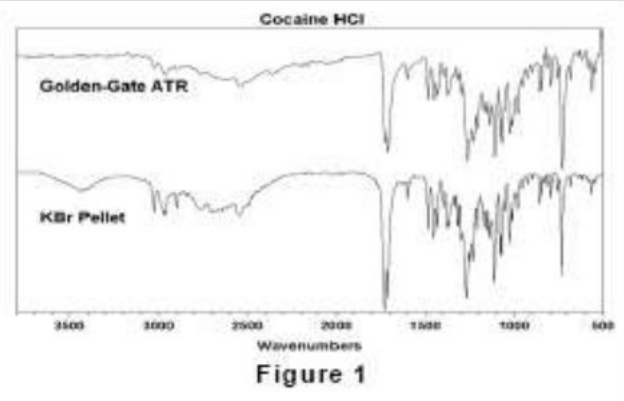

Figure 1

This is illustrated in Figure 1, which shows both transmission and ATR spectra of cocaine HCl.

However, despite the changes in peak intensity, peak locations can be verified with transmission spectra. Sample spectra can also be searched against a digital database of ATR spectra[2] and positive identification can be obtained for controlled narcotics and synthetic analogs[3].

Experiment and Results

Spectra were collected using a Golden Gate Diamond ATR accessory equipped with ZnSe lenses (optional KRS-5 lenses are available to increase the spectral range) and a single-reflection diamond ATR element.

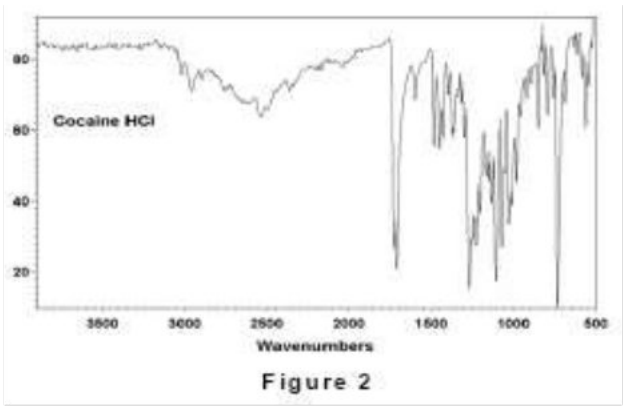

Figure 2

The accessory is equipped with a sapphire clamping anvil that can be removed for cleaning. A background spectrum of the accessory was collected before every sample scan to ensure no sample cross contamination. A small amount of the neat sample was placed onto the ATR crystal and the anvil was hand-tightened to the preset pressure.

FT-IR spectra of 36 scans at 4 cm-1 resolution were co added and averaged to obtain the single-beam background and sample spectra. Total sampling time was approximately 2-5 minutes per sample, including accessory cleanup and background collection. Samples were analyzed sequentially with no sample preparation.

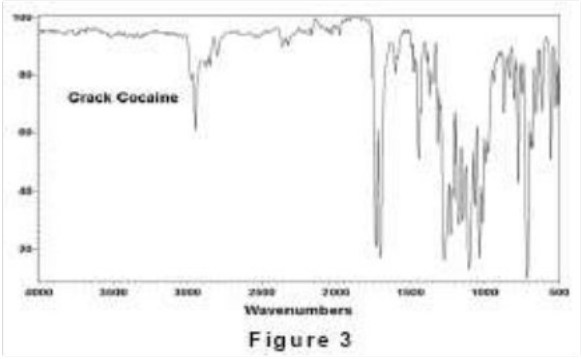

Figure 3

On occasion, only a small amount of sample is available for analysis. Using the Golden Gate micro-ATR, spectral data can be collected using sample amounts of 20-30 milligrams and even single grains of sample can be analyzed.

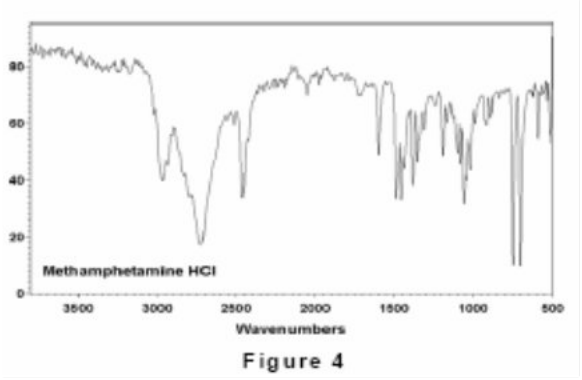

Figure 4

Figures 2 and 3 are a comparison of the spectra for samples of cocaine HCl and the free base of cocaine (crack cocaine), respectively.

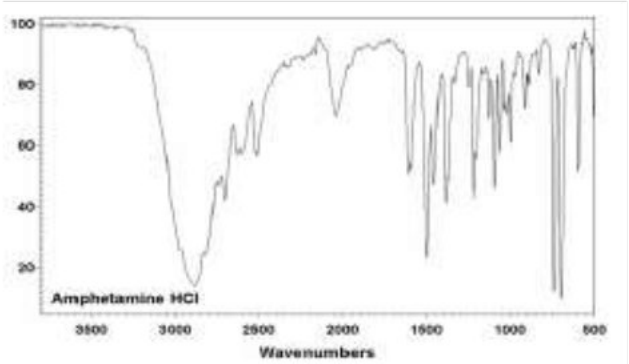

Figure 5

Closely related synthetic derivatives of controlled substances or 'cutting agents' used to extend quantity must be readily distinguished. Figures 4 and 5 are spectra of methamphetamine and amphetamine, respectively. Figures 6 and 7 are spectra of ephedrine and caffeine.

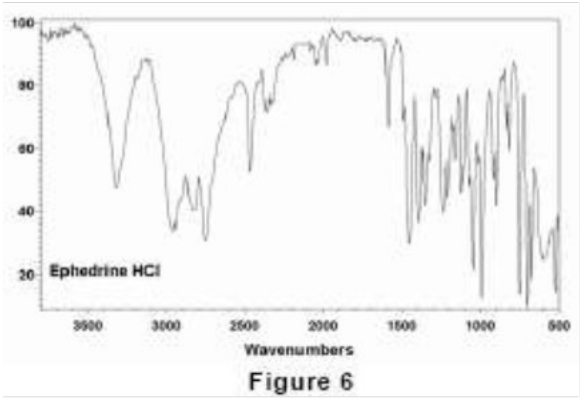

Figure 6

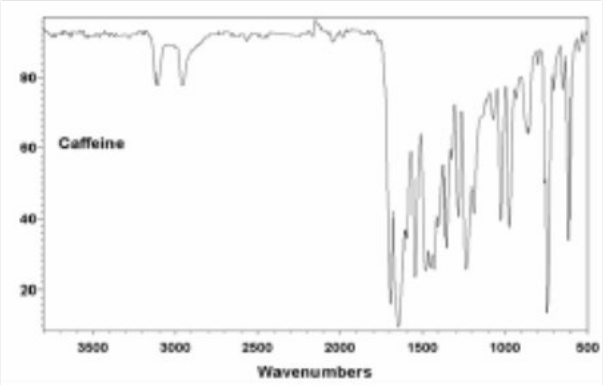

Figure 7

Conclusion

The Golden-Gate Diamond ATR system is a simple, easy-to-use accessory for the analysis of drugs of abuse. The ATR technique requires no sample preparation, is rapid and very reliable for the characterization of neat samples. The method is non-destructive and can be used to analyze a minimal amount of sample.

References

1. Gilby, A. C., Cassels, J., and Wilks, P. A., Applied Spectroscopy, 24(5), 1970.
2. Koulis, C. V., Hymes, K. J., Rawlins, J. L. Journal of Forensic Sciences, 2000, 45, 876.
3. The ATR library of 455 compounds is available for download on the Illinois State Police web-site at: http://www.state.il.us/isp/forensic/druglibrary.htm

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Specac Ltd
River House
97 Cray Avenue, Orpington
Kent, BR5 4HE.
United Kingdom
T: +44 (0) 1689 873134
F: +44 (0) 1689 878527
E: sales@specac.co.uk

Specac Inc
414 Commerce
Drive, #175
Fort Washington, PA
19034, U.S.A.
T: 1 866 726 1126
E: sales@specac.com