Not all FT-IR Spectrometers are the Same: High Energy Throughput

APPLICATION BRIEF

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Introduction

Varian's FT-IR spectrometers are noted for their outstanding performance as characterized by the amount of infrared energy in the sample compartment. The increased energy in the sample compartment translates to higher signal to noise ratios (S/N), which ultimately can mean a greater sensitivity or ability to detect small differences in samples. While S/N is a measure of system performance, it is not the best measure for the quality of spectra obtained on real world samples. Manufacturers tend to obscure how their results are obtained and under what conditions they are acquired. Varian's systems are more accurately measured by providing the actual energy at the sample. The energy varies by system choice. This application brief shows the "real world" performance advantage of Varian's Scimitar series over another manufacturer's product offering.

Experimental Details

The following experiment was conducted with two spectrometers. The first spectrometer was Varian's Scimitar 1000, which is a mid-infared spectrometer derived from the Excalibur^{TM} family of spectrometers. The second spectrometer was a leading manufacturer's product offering. In each case, a diffuse reflectance sampling accessory optimized to the manufacturer's spectrometer was used. The first experiment consisted of filling the diffuse reflectance sample holder with KBr powder and collecting a hundred percent line (HPL) spectra using KBr as the background and the sample. In each case, the data collection parameters were set so that identical conditions existed between the two instruments. The table below summarizes these conditions.

Spectrometer	Apodization	# Data Points	Res. cm^{-1}	#Co-added Scans	Total Scan Time
Scimitar Series	Happ Genzel	8479	3.354	10	20 sec.
Other	Happ Genzel	8480	4.000	16	20 sec.

Results and Discussion

Figure 1 shows the results of the HPL tests. The spectra are displayed over the region of 1900-1500 cm^{-1}. The blue trace is the spectrum from the Scimitar while the red trace is the spectrum from the other manufacturer's spectrometer. These results show that the Scimitar exhibits far less "spectral noise" under these scan conditions.

The second experiment consisted of obtaining the infrared spectra of crushed aspirin tablets that were spiked with caffeine. For one sample, two 325 mg aspirin tablets were crushed and diluted with KBr. For the other sample two 325 mg aspirin tablets were crushed and 1% caffeine by weight was added to the aspirin and this mixture was diluted with KBr. Infrared spectra of the aspirin and aspirin caffeine samples were acquired using the same conditions for the HPL experiment that was described above.

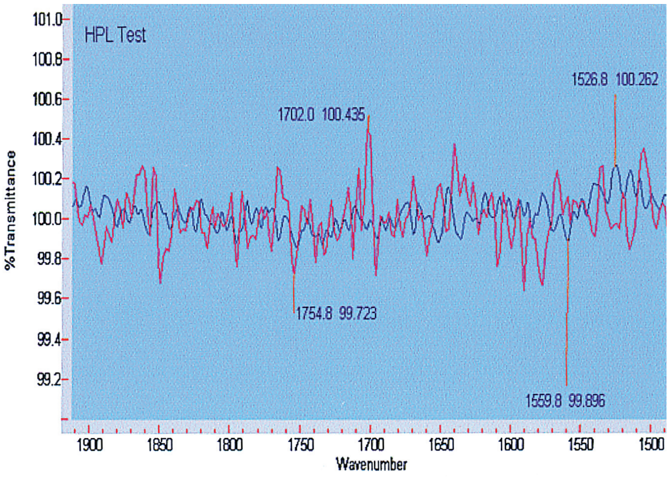
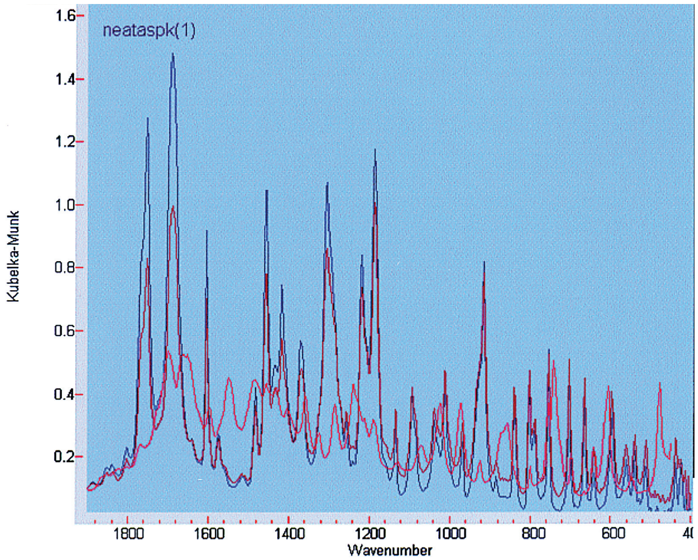


Figure 1. Results of the HPL tests.

Results and Discussions (continued)

One result of higher signal to noise is the ability for the instrument to detect small changes in material composition. Figure 2 and 3 illustrate these results.

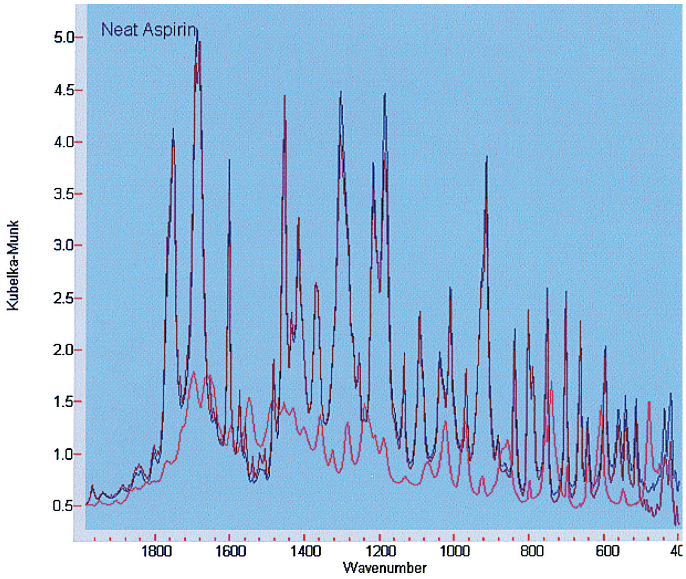


In Figure 2, the blue trace is the spectrum of aspirin and the purple trace is the spectrum of 1% caffeine in aspirin, while the red spectrum is from a caffeine sample. Note that it is not possible to distinguish the 1% caffeine in aspirin sample from the aspirin sample. These spectra were acquired on another manufacturer's spectrometer.

Figure 2. Spectra of aspirin (blue), aspirin with 1% caffeine (purple), and caffeine (red) from another manufacturer's spectrometer.

In Figure 3, similar results are shown from the Scimitar spectrometer. With this spectrometer it is possible to detect differences between the 1% caffeine in aspirin sample and the aspirin sample. This is most apparent when looking for the caffeine peak at 1650 cm^{-1}. In Figure 3, this is observed as a shoulder on the aspirin/caffeine spectrum, while it is not possible to see this shoulder in the aspirin/caffeine spectrum from Figure 2.

Figure 3. Spectra of aspirin (blue), aspirin with 1% caffeine (purple), and caffeine (red) from the Scimitar spectrometer.



Conclusion

The data presented in this application brief shows that not all spectrometers are alike. Indeed, the Varian Scimitar spectrometer's superior throughput translates to higher signal to noise ratio than the competition's products. A higher signal to noise ratio means an imporvement in the ability to detect small changes in sample composition.

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