

Tech Note

The Difference Between VFA and FT-IR Spectra

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The basic characteristics of variable filter array (VFA) spectrometers, both near- and mid-infrared, available from several manufacturers, make them well suited for routine infrared analysis applications outside and inside the laboratory. Although the infrared data gathered by a VFA spectrometer is similar to that obtained from an FT-IR instrument, it differs in one key respect — resolution. In the mid-IR region, FT-IR spectra usually are recorded at resolutions between 0.5 cm^{-1} and 8 cm^{-1} . A VFA spectrometer with 64 pixels has a theoretical resolution of 16 cm^{-1} . Because of crosstalk from pixel to pixel, both thermal and optical, the resolution is reduced further to the neighborhood of 50 cm^{-1} .

What effect does low resolution have upon the performance of a VFA spectrometer? To answer this question, we have used a VFA spectrometer in several different applications to determine the effect, if any, of low resolution.

Raw material verification. A company uses a solvent that comes in three isomers, each specific to a different process. Sending a sample to the laboratory can take over an hour for verification, delaying the offloading of the material. Figure 1 shows VFA spectra of the three isomers. Even though the spectral information in the VFA spectra is considerably less than that of FT-IR traces, there is enough data from the VFA spectrometer to verify the isomer in the shipment. Because a VFA spectrometer has no moving parts and no free air path, it is unaffected by atmospheric absorptions and can be situated at the receiving dock. In less than 5 min, the incoming raw material can be verified and off-loaded to the correct location.

Process monitoring. In a process, a material that has an absorption band “A” between 8.5 and 9 μm (Figure 2) converts to a material that has band “B” at 7.0 μm . The reaction can take several hours. The figure shows spectra periodically taken by the VFA instrument situated close to the production line, which follow the switch from “A” to “B”. Again, in this

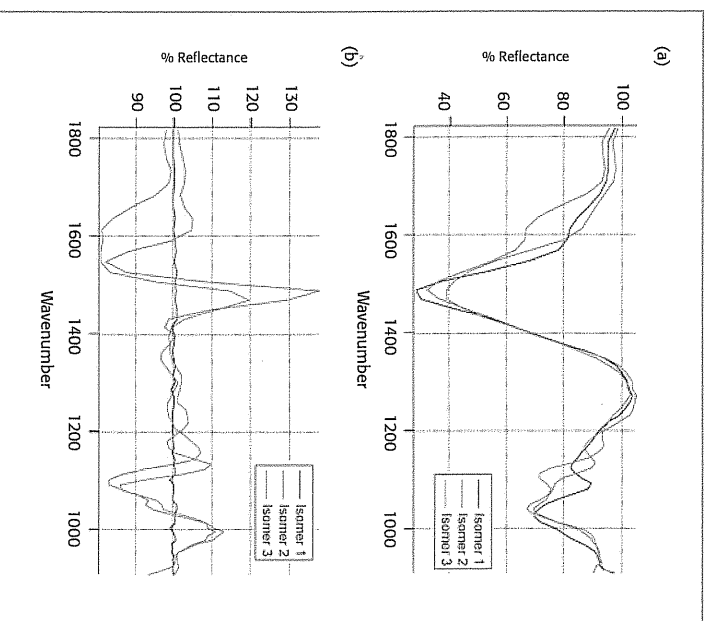


Figure 1. (a) Infrared spectra of three isomers. (b) Using Isomer 1 as a reference, a spectrum of Isomer 1 produces a straight line while the spectra from the other two isomers show deviations from a straight line.

situation, the resolution is sufficient to tell when a reaction is complete.

Flexible film manufacturing. There are many areas in flexible film manufacturing in which an onsite test is invaluable.

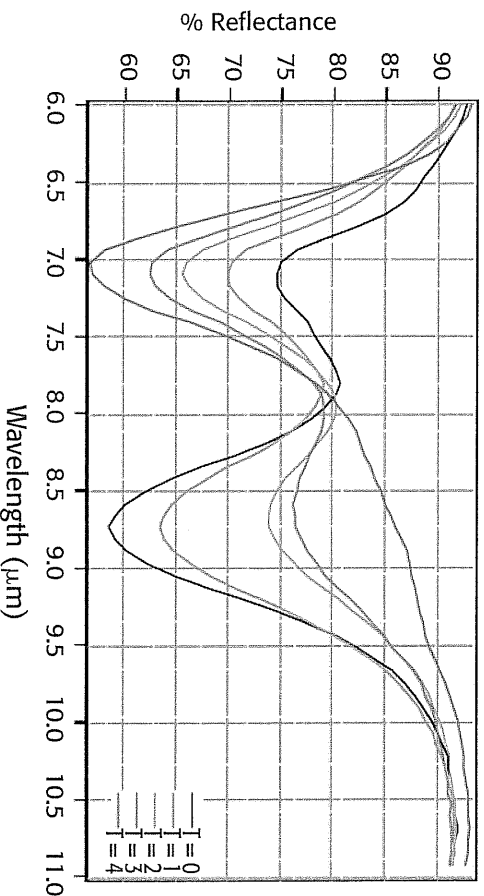


Figure 2. Following a reaction. As the reaction progresses, the band between 8.5 and 9 µm decreases to be replaced by the band at 7.0 µm.

With multilayer films, rolls of film are laminated together with individual rolls, often having different top and bottom materials. Figure 3 shows spec-

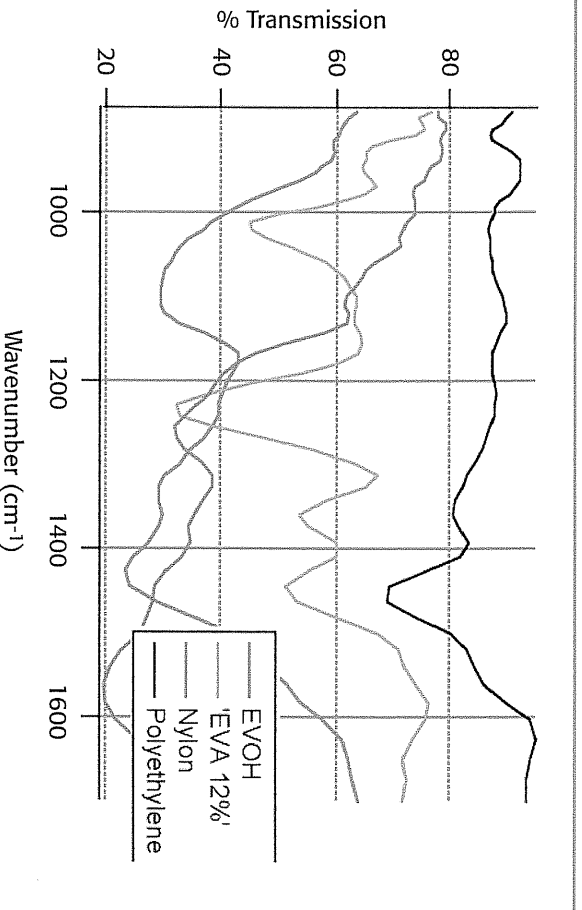


Figure 3. Spectra of common materials used in flexible film production.

ent it in the right direction for lamination. In the warehouse, rolls of finished films can be verified on-site before shipment to ensure that the customer is receiving the desired product. Another application involves measuring an inside layer thickness, such as nylon, in a multilayer film. Nylon has an absorbance different from the spectra of the outside polyethylene layers, which can be distinguished with a lower resolution VFA spectrometer.

FT-IR Spectra

“White powder” verification. Partly as a result of 9/11, and partly because materials are being examined frequently for identification purposes, mid-IR FT-IR spectrometers have become widely used for this purpose to the extent that libraries containing thousands of spectra of known materials have been constructed. Is it feasible to use a VFA spectrometer to search the libraries for identification purposes?

The spectra of common pharmaceutical products shown in Figure 4 are a good example of the differences between VFA spectra and FT-IR spectra. While each VFA spectrum is distinctly different from the others, each also is quite different from its FT-IR counterpart. Because of these substantial differences, it appears to be impractical to compare spectra from FT-IR libraries directly.

On the other hand, if one examines the VFA spectra, it becomes apparent that each product has a characteristic VFA spectrum, sometimes more readily identifiable than its FT-IR spectrum, so libraries of VFA spectra could serve to identify various groups of materials. For example, a pharmaceutical company might use one of the VFA spectral libraries VFA spectra could be created. **Author:**

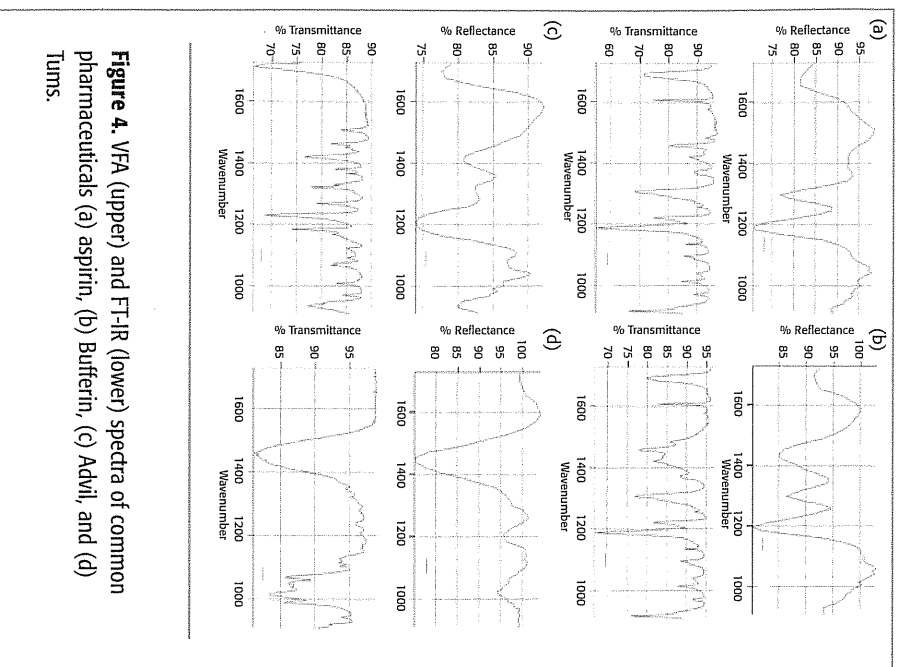


Figure 4. VFA (upper) and FT-IR (lower) spectra of common pharmaceuticals (a) aspirin, (b) Bufferin, (c) Advil, and (d) Tylenol.

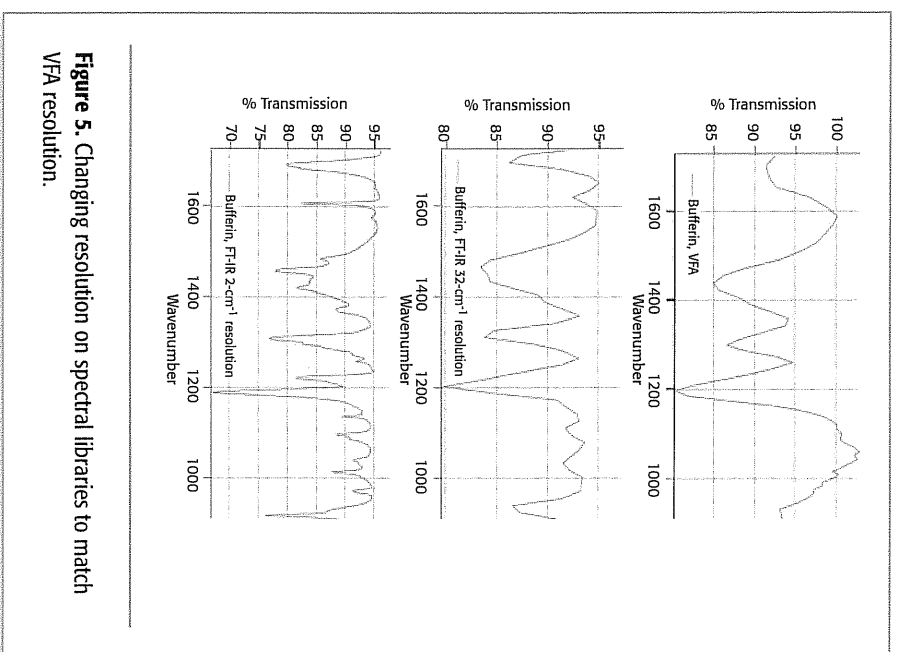


Figure 5. Changing resolution on spectral libraries to match VFA resolution.

Please clarify this sentence!

While it does not appear that the VFA spectrometer will replace the FT-IR instrument as a general purpose unknown material identifier, it can be used for this purpose when a relatively small number of materials is involved. Because VFA spectrometers are small, rugged, and usually contain no moving parts or exposed optical paths, they can be practical alternatives to FT-IR instruments when applicable.

It is possible to degrade FT-IR spectra from spectral libraries to lower resolution, as in Figure 5, so that they tend to match VFA spectra. However, in so doing, search programs would be far less specific and generally would produce a number of possible hits rather than one or two.

Low Resolution Effects Can Be Positive

From the examples presented here, it is apparent that low-resolution mid-IR data is not necessarily a deterrent and often can have a positive effect. As the examples show, low-resolution spectra frequently contain gross differences between spectra of materials, so that visual verification of materials is feasible. Automatic identification from a VFA spectra library also is feasible. Although FT-IR spectra can contain much more detail, visual differences tend to be less apparent, and therefore, require a more detailed systematic evaluation for positive identification. Obviously, both high-resolution FT-IR

spectra and low-resolution VFA spectra are useful, depending upon the application. ■

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