

Figure 1. The ConcentratIR2™ multiple-reflection ATR accessory.

## Analysis of Edible Oils by Multiple Reflection ATR

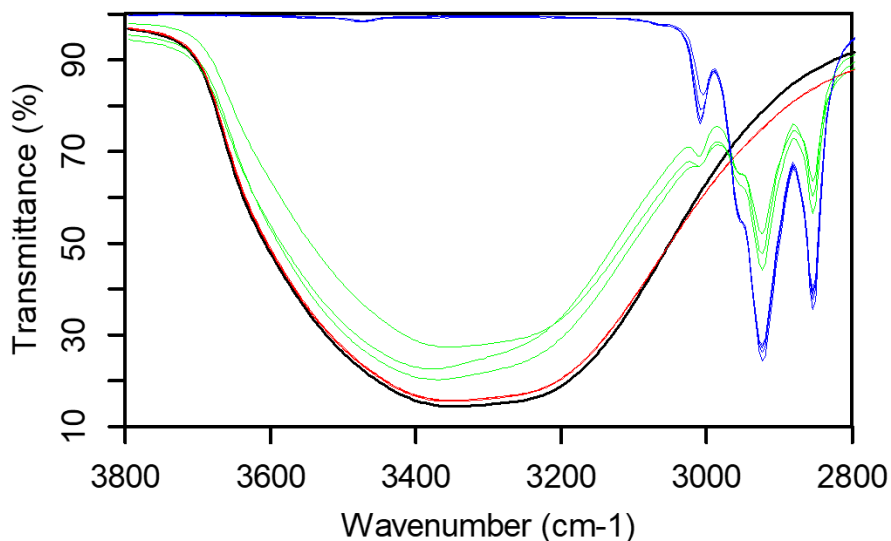
### INTRODUCTION

Attenuated total reflectance (ATR) IR spectroscopy allows for the analysis of small amounts (as little as 10  $\mu\text{L}$ ) of strongly IR-absorbing samples, such as aqueous solutions. This application note demonstrates the ability of the Harrick [ConcentratIR2™](#), a multiple reflection diamond ATR, to analyze and identify aqueous, oil-based, and mixed oil/aqueous solutions using a minimal amount of sample.

### EXPERIMENTAL

All IR spectra were collected on a commercial FT-IR spectrometer with the ConcentratIR2™ (see Figure 1) placed in the sample compartment, using a DTGS KBr detector. All spectra were produced from 32 averaged scans at a resolution of 8  $\text{cm}^{-1}$ . The gain was set to 8, the aperture was set to 100 (fully open), and spectra were collected in the range 4000-400  $\text{cm}^{-1}$ . The spectrometer and accessory were purged with filtered air (water and carbon dioxide removed) that was produced by a Parker Balston Model 75-62 FT-IR Purge Gas Generator at 40 SCFH.

Figure 2. Spectra of aqueous solutions (red), oils (blue), mixed solutions (green), and water (black) over the spectral range 3800-2800  $\text{cm}^{-1}$ .



The samples investigated were all dressings, oils, and vinegars available at most grocery stores. Each sample was analyzed by placing one drop on the diamond ATR crystal.

## RESULTS AND DISCUSSION

The samples used can be divided into three main categories: aqueous/dilute acid solutions, oils, and mixtures of aqueous solutions and oil. The distilled white vinegar, Holland white vinegar, and Progresso Red Wine Vinegar are the aqueous/dilute acid solutions, shown in red. The Berio olive oil, canola oil, vegetable oil, and Wesson oil are the oils, shown in blue. The Hellman's Mayonnaise, Hidden Valley Dressing, and Spectrum Canola Mayonnaise are mixtures, shown in green. A spectrum of pure water is provided for reference, shown in black.

The spectra in each group are very similar and share a number of key features. Figure 2 shows the spectral range 3800-2800  $\text{cm}^{-1}$  where the three different groups can clearly be identified. The aqueous/dilute acid solutions have only the broad  $\text{H}_2\text{O}$  band, while the oils lack the  $\text{H}_2\text{O}$  band but have strong peaks in the 3000-2800  $\text{cm}^{-1}$  range, characteristic of

C-H bonds. The mixed solutions have both the  $\text{H}_2\text{O}$  band and the C-H bands.

Figure 3 shows the spectral range 1800-1000  $\text{cm}^{-1}$ . The aqueous solutions have the characteristic  $\text{H}_2\text{O}$  band around 1650  $\text{cm}^{-1}$ , as well as bands at 1400  $\text{cm}^{-1}$  and 1290  $\text{cm}^{-1}$ , which, along with the aforementioned C-H bands, clearly distinguish them from pure water. The oils do not have the  $\text{H}_2\text{O}$  band but rather have a strong, sharp peak at around 1750  $\text{cm}^{-1}$ , characteristic of C=O bonds. They also have peaks at 1470  $\text{cm}^{-1}$  and 1170  $\text{cm}^{-1}$  that are not present in the aqueous solutions. The mixed solutions again share features of both the aqueous solutions and the oils. They have the  $\text{H}_2\text{O}$  band at 1650  $\text{cm}^{-1}$ , as well as the carbonyl band at 1750  $\text{cm}^{-1}$ . They also share the bands found in oil at 1470  $\text{cm}^{-1}$  and 1170  $\text{cm}^{-1}$ .

## CONCLUSIONS

The Harrick ConcentratIR2™ ATR accessory allows for rapid analysis of small amounts of both aqueous and non-aqueous liquids. Comparisons were easily made between solutions containing only water, only oil and both water and oil.

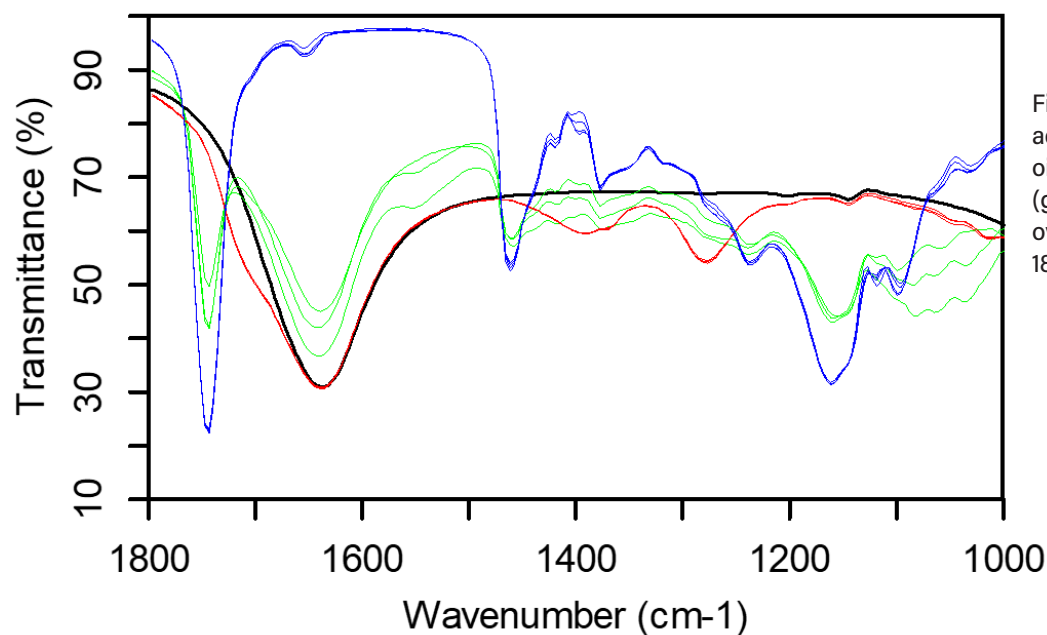


Figure 3. Spectra of aqueous solutions (red), oils (blue), mixed solutions (green), and water (black) over the spectral range 1800-1000  $\text{cm}^{-1}$ .