

KINETIC STUDY USING MID-IR FIBER OPTICS



Figure 1. The FiberMate2 connected to MultiLoop-MIR fiber optic ATR probe.

INTRODUCTION

This work investigates the interaction of 70% isopropyl alcohol with acetone. After mixing, the relative concentrations of the three components – water, isopropyl alcohol and acetone – change until equilibrium is achieved. This interaction is studied here using a mid-infrared fiber optic liquid probe.

EXPERIMENTAL

The experiment was carried out using a commercial FTIR spectrometer with Harrick's FiberMate2 fiber optic coupler and MultiLoop-MIR fiber optic ATR probes. The spectrometer was configured with an MCT/A detector and KBr beam splitter. Spectra were signal averaged over 12 scans, with an 8 cm^{-1} resolution and an aperture of 100%. Measurements were taken using the CIR ATR probe in the range of $4000\text{--}1500\text{ cm}^{-1}$ and with the PIR probe over the $2000\text{--}600\text{ cm}^{-1}$ range. The background measurements were collected using the clean ATR probe. Sample measurements were taken with the probe dipped into a beaker which contained the liquid sample. To eliminate changes in the spectra due to the curvature of the fiber, the probe was clamped in position.

The beaker was filled with 90 ml of acetone and a sample spectrum collected. Then 10 ml of 70% isopropyl alcohol (IPA) was added. A spectrum was collected immediately after mixing and periodically for the next 40 sec. as the mixture was gently swirled.

RESULTS AND DISCUSSION

The ATR spectra collected with the CIR fiber, over the $4000\text{--}1500\text{ cm}^{-1}$ spectral range are shown in Figure 2. The most notable changes are those to the --O--H and --C--H stretches. The growth in the --O--H stretch is examined in more detail in Figure 3, where the spectrum of acetone was subtracted from the spectra of the mixtures, to remove the band at 3412 cm^{-1} , and then the area under the --O--H band was calculated. The result shows a fast initial increase in the --O--H content from IPA/water which then tails off with time as the system approaches equilibrium. In acetone, the C-H stretching band at 2970 cm^{-1} is weaker than the band at 3005 cm^{-1} . Over time, the intensity of the 2970 cm^{-1} band increases relative to the band at 3005 cm^{-1} , indicating that the acetone is evaporating more quickly than IPA/water.

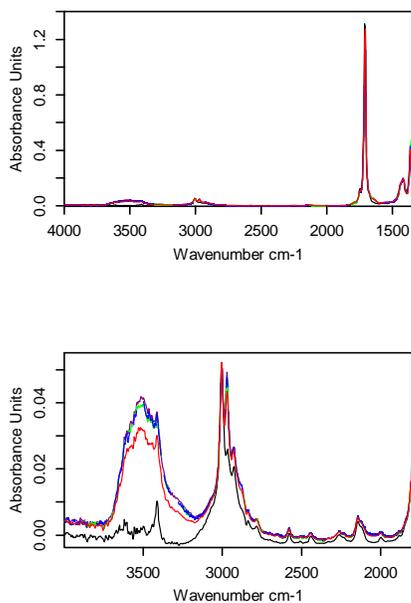


Figure 2. ATR spectra of the acetone-IPA mixture after 27 sec (red), 222 (blue), 233 (green) and 263 (purple) seconds after mixing, shown relative to acetone (black). Top: full spectrum. Bottom: expanded view.

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Figure 4 shows the spectra collected using the PIR fiber in the fingerprint region. The band at 1642 cm^{-1} grows with time, indicating the increased concentration of water. The bands at 945 cm^{-1} and 816 cm^{-1} from the isopropyl alcohol decreases over time, indicating that the isopropyl alcohol is also evaporating, albeit more slowly than acetone.

This study demonstrates the feasibility of carrying out kinetic studies in the mid-infrared using the fiber optic probes, such as the Multi-Loop-MIR.

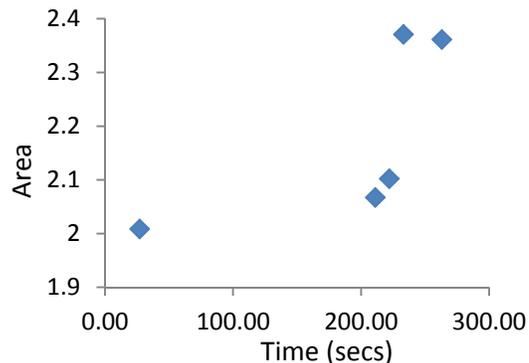


Figure 3. Area of the -O-H band as a function of time.

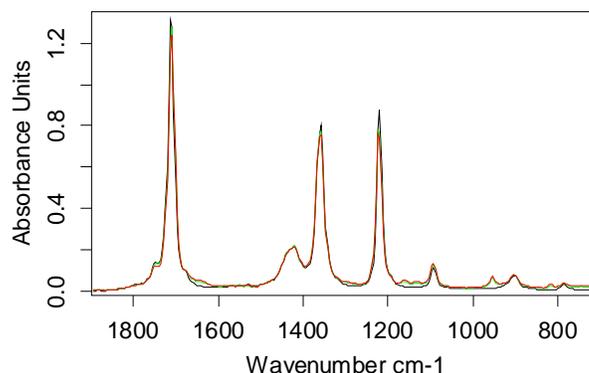


Figure 4. ATR spectra of the acetone-IPA mixture immediately after mixing (red) and after ~ 2 min. (green), shown relative to acetone (black).



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