# Assessing Formulation in Polymeric Materials by ATR/FTIR

## Introduction

Polyurethane may take many physical forms such as foam, soft rubber, or rigid plastic. It is made by reacting a monomer containing isocyanate groups with a monomer containing alcohol groups in the presence of a catalyst. The material properties of polyurethane products are dependent on the isocyanate and the alcohol groups, and the ratios of each used during the reaction. Therefore, it is desirable to have a fast and reliable method to evaluate the accuracy of formulations as a quality assessment tool. ATR/FTIR offers such a solution.

## Materials and Methods

Semi-rigid polyurethane samples were analyzed by ATR/FTIR. These samples contained varying ratios of isocyanate to alcohol monomers. The PIKE MIRacle ATR accessory (Figure 1) was used in this investigation. The polyurethane sample was placed over the ZnSe crystal, and high pressure was applied. Spectral range covered 4000 to 520 $cm^{-1}$. Spectra were collected at 4 $cm^{-1}$ spectral resolution utilzing a 1 minute data collection time. No sample preparation was required. Samples were run at room temperature.



**Figure 1. PIKE MIRacle.**

## Results

Sample spectra are shown in Figure 2. Spectral differences between sample formulation are observed at 2260 $cm^{-1}$, the isocyanate absorbtion band (Figure 3). Due to the high throughput of the MIRacle accessory, providing the highest signal-to-noise ratio, these bands are easily quantified. In this specific application, this absorption may be used to determine the degree of excess isocyanate monomer remaining in the system after the reaction is complete, which is an indicator of utilizing the proper monomer ratio in the formulation.
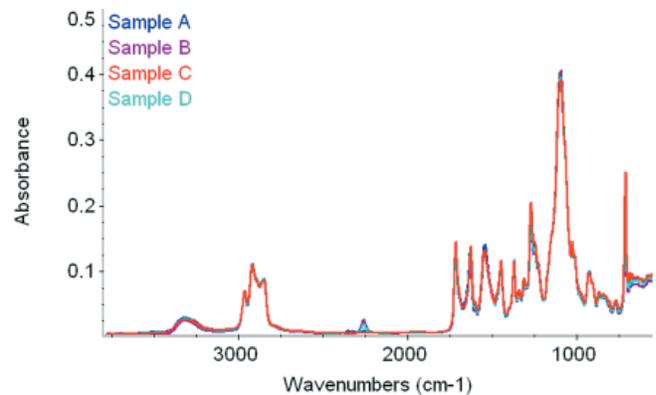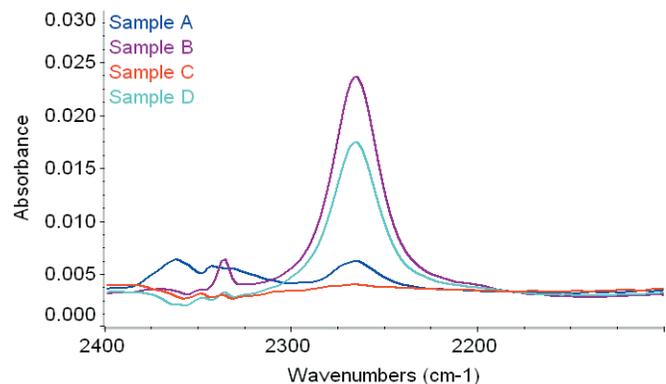


**Figure 2. Polyurethane spectra.**



**Figure 3. Polyurethane spectra expanded view of isocyanate absorbtion band.**

## Summary

The high throughput of the MIRacle ATR accessory allows spectroscopy to be implemented as an important tool to evaluate formulation accuracy in reactive products.