Applications of Mixture Analysis to FT-IR Spectra of Multi-Component Polymeric Systems

Dana Garcia,[1] and Marie Scandone,[2]

(1) Arkema Inc. 900 First Avenue, King of Prussia, PA 19406-0936, (2) Bio-Rad Laboratories, Inc., Informatics Division, Two Penn Center Plaza, Suite 800, 1500 John F. Kennedy Blvd., Philadelphia, PA 19102-1737

Introduction

IR spectral identification of multi-component samples is a challenging process:

- Highly overlapping peaks
- Lack of specific component knowledge
- Assignment of functional groups to a specific component
- Time intensive one-component-at-a-time spectrum analysis

KnowItAll® mixture analysis effectively addresses IR spectral identification of multi-component samples.

Mixture analysis is a mathematical process to extract:

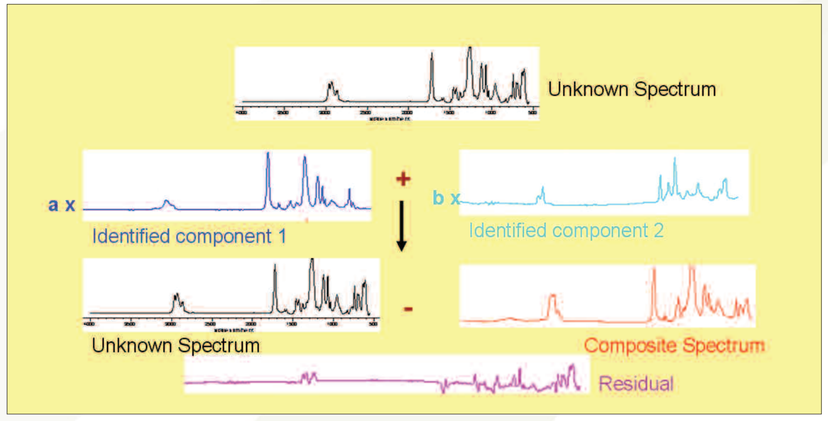
- Combinations of IR spectra in a library database
- Simultaneously minimizing the residual relative to the unknown IR spectrum

Mixture analysis results:

- Provide a series of potential unknown component IR spectra for evaluation
- Improve data mining efficiency
- Simplify search results evaluation

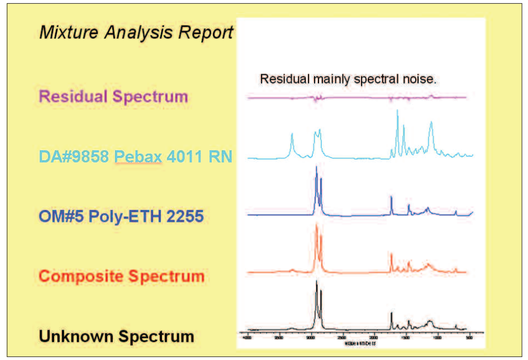
Mixture Analysis

Algorithm for Spectral Fitting:
Finding combinations of database IR spectra that minimize residual.



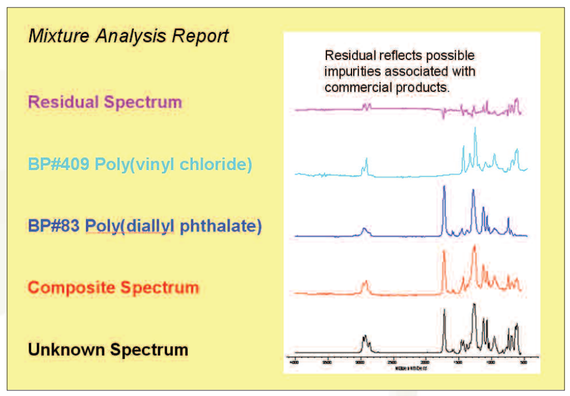
Residual intensity comparible or smaller than obtained through standard spectral subtraction.

Example 1. Two Component Polymeric System



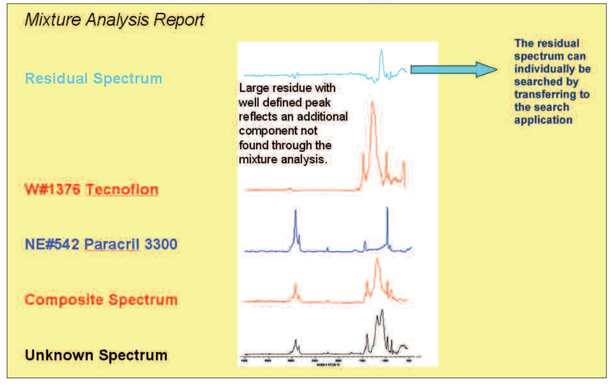
Component DA#9858 could not be identified through simple searching.

Example 2. Polymer Plasticizer Blend

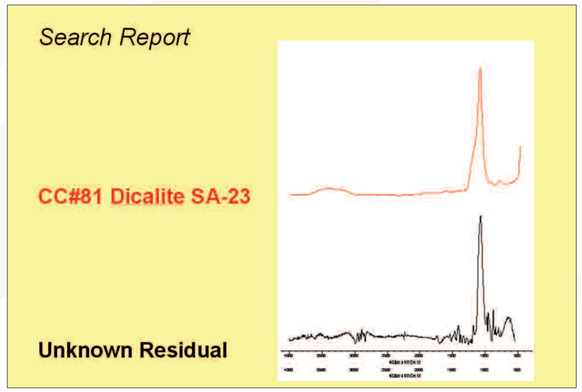


Both components identified in a single step.

Example 3a. Three Component Polymeric Filler System



Example 3b. Three Component Polymeric Filler System Filler Identification



A combination of mixture analysis and simple search identified all three components of the formulation:

- Tecnoflon® & Paracril® 3300 & Dicalite® SA-23

Conclusions

IR spectral identification of multi-component samples lends itself to a combination approach using mixture analysis and simple spectral search.

High degree of module interconnectivity.

Integrated with all other functionalities of KnowItAll®.

- Individual module provide partial answers
- In totality a systematic and efficient analysis

Applicable to a wide variety of spectral identification problems.