

Usefulness of Mixture Analysis with Spectra Genius Mixture Master

Ryosuke Sasaki, Hideyuki Masui
1-16-27 Minaminakahuri, Hirakata-Shi, 573-0094, Japan
Email: sasaki@stjapan.co.jp

Mixture Analysis (MA) attempts to determine the components of a mixture spectrum. A mixture spectrum is a spectrum of two or more compounds in a sample; MA answers two questions: (1) what is the spectrum of the individual components, and (2) what is the ratio of those components. MA is solved by (1) using repeated library searches to identify the components of a mixture and (2) using linear regression to determine the contribution of the components to the mixture, although a condition is required that the library must always contain the correct answer or similar compounds. Unlike multivariate analysis, MA does not require a large amount of data, but only a library, MA can analyze the third component and, if necessary, the fourth component. Known components can be specified in advance during the analysis, which increases the accuracy of predicted components and concentrations. The ability to specify known components is expected to be used in the field of foreign material analysis and material development. Liquid samples of mixtures of the four components were evaluated by analyzing the actual spectral data measured by the ATR method with an FT-IR spectrometer.