Application Note AN-RS-006

Differentiation between isopropyl alcohol from various manufacturers

This Application Note shows the rapid, nondestructive identification of isopropyl alcohol from two manufacturers using Raman spectroscopy following the creation of a suitable library. The measurements with the handheld Raman spectrometer Mira M-1 require no sample preparation and provide immediate results that identify the samples unambiguously.

INTRODUCTION

Organic solvents like isopropyl alcohol are required in the production of many beauty and cosmetic products, paints, fragrances, and in synthesis reactions – the latter in particular in pharmaceutical applications. In this work, isopropyl alcohol samples from two different suppliers were analyzed and the differences in the spectra were investigated. Unexpectedly, the spectra showed some differences, allowing a supplier-specific identification.

EXPERIMENTAL

All spectra were measured using the Mira M-1 Raman spectrometer in auto-acquisition mode, i.e., integration times were determined automatically. A laser wavelength of 785 nm and the Orbital-Raster-

Scan (ORS) technique were used. The isopropyl alcohol samples were analyzed in vials using the vial holder attachment of the Mira M-1.

RESULTS AND DISCUSSION

Two different suppliers of isopropyl alcohol were evaluated. Due to the visible differences in the spectra indicating a possible contamination of the samples

the Raman spectroscopic distinction was possible (see Figure 1).



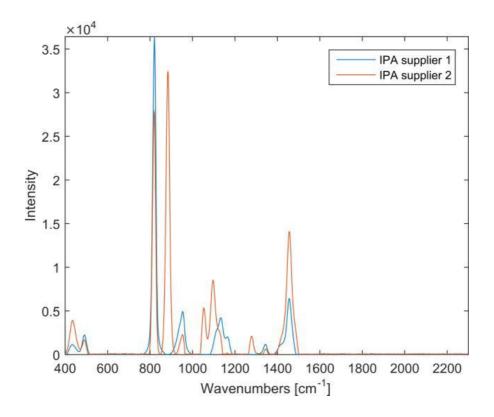


Figure 1. Spectra of isopropyl alcohol (Supplier 1 and 2) superimposed with a spectrum of ethyl alcohol

The peaks at $1400-1470~{\rm cm}^{-1}$ correspond to the asymmetric vibrations of $\delta({\rm CH_2})$ and $\delta({\rm CH_3})$. Between $600-1300~{\rm cm}^{-1}$, aliphatic chain vibrations for $\upsilon({\rm CC})$ can be found. In both samples of isopropyl alcohol, peaks in those areas can be observed.

Changes come up when focusing on the peaks at 883, 1049, 1095, and 1276 cm⁻¹, since those peaks, according to literature, suggest the presence of ethyl alcohol in the sample (see **Figure 2**).

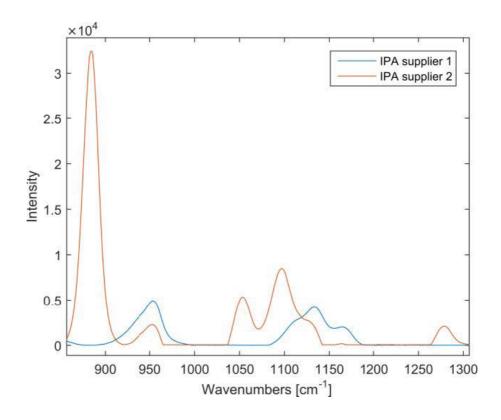


Figure 2. Differences between the isopropyl alcohol spectra.

CONCLUSIONS

Comparing the spectra of the two isopropyl alcohol samples, it becomes obvious that there is ethyl alcohol in the isopropyl alcohol sample of supplier 2. With Mira M-1, it was possible to distinguish the

different suppliers, proving that Mira M-1 is suited for the identification of incoming raw materials such as solvents and alcohols.

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CONFIGURATION



MIRA P Advanced

The Metrohm Instant Raman Analyzer (MIRA) P is a high-performance, handheld Raman spectrometer used for rapid, nondestructive determination and verification of different material types, such as Pharmaceutical APIs and excipients. Despite the small size of the instrument, the MIRA P has a ruggedized design and features a high-efficiency spectrograph design equipped with our unique Orbital-Raster-Scan (ORS) technology. The MIRA P is fully compliant with FDA 21 CFR Part 11 regulations.

The Advanced Package includes an attachment lens for analyzing materials directly or through containers (laser class 3b), as well as a vial holder attachment for analyzing samples contained in glass vials (laser class 1).

