Handheld Raman for Acid Attack Prevention

Identification of acids through a novel plastic container

Summary

Acid throwing, a historical method for retribution against women, has become more prevalent in recent years. In 2017, the United Kingdom reported such incidents averaging twice per day. Concentrated acids and other corrosive substances have emerged as modern tools of social violence. Aggressors use common plastic containers with small openings that create a powerful directional spray, such as lemon or lime juice squeeze bottles.

Detection and regulation of acids may help to prevent such attacks. MIRA (Metrohm Instant Raman Analyzer) DS is an ideal solution for forensic investigation of suspicious containers. Large libraries, automated data collection and analysis, through-container interrogation, and a rugged, compact form factor all combine in MIRA DS to address this modern threat. This Application Note contains a discussion of how strong acids and corrosive bases appear in the Raman spectrum. Sulfuric and phosphoric acids were chosen for analysis through the plastic of a squeeze bottle, due to their highly corrosive nature and common usage.

Configuration

2.926.0020 - MIRA DS Advanced

The Metrohm Instant Raman Analyzer (MIRA) DS is a ruggedized, high-performance, handheld Raman spectrometer used for rapid, nondestructive determination of illicit materials, e.g. drugs, explosives, starting materials, and hazardous agents. Despite the small size of the instrument, MIRA DS is extremely rugged and features a high-efficiency spectrograph equipped with our unique Orbital-Raster-Scan (ORS) technology.The Advanced package includes the Library of illicit materials, calibration standard, universal attachment for analyses in bottles or bags or for direct analysis, and the right-angle attachment, ideal for running samples on a surface and/or in a bag. Class 3B operation.

6.07502.000 - Vial Holder

Vial holder attachment for Mira M-3/P/DS. Accommodates 15 x 26 mm glass vials.

6.07505.000 - Attachment lens (LWD)

Long distance point-and-shoot Adapter (LWD) for the Mira M-3/P/DS Advanced Package with a focal length of 7.6 mm. Class 3B operation.

Experiment

Raman spectra of eight strongly corrosive acids and bases were collected to establish the suitability of Raman spectroscopy as a material identification technique.

Sample preparation

Most acids and bases were sampled in their concentrated state. Distilled water was used to prepare acid dilutions. Sodium hydroxide was prepared as a saturated aqueous solution. All samples were placed in glass vials and inserted into the Vial Holder attachment on MIRA DS for initial analysis (**Figure 1**).

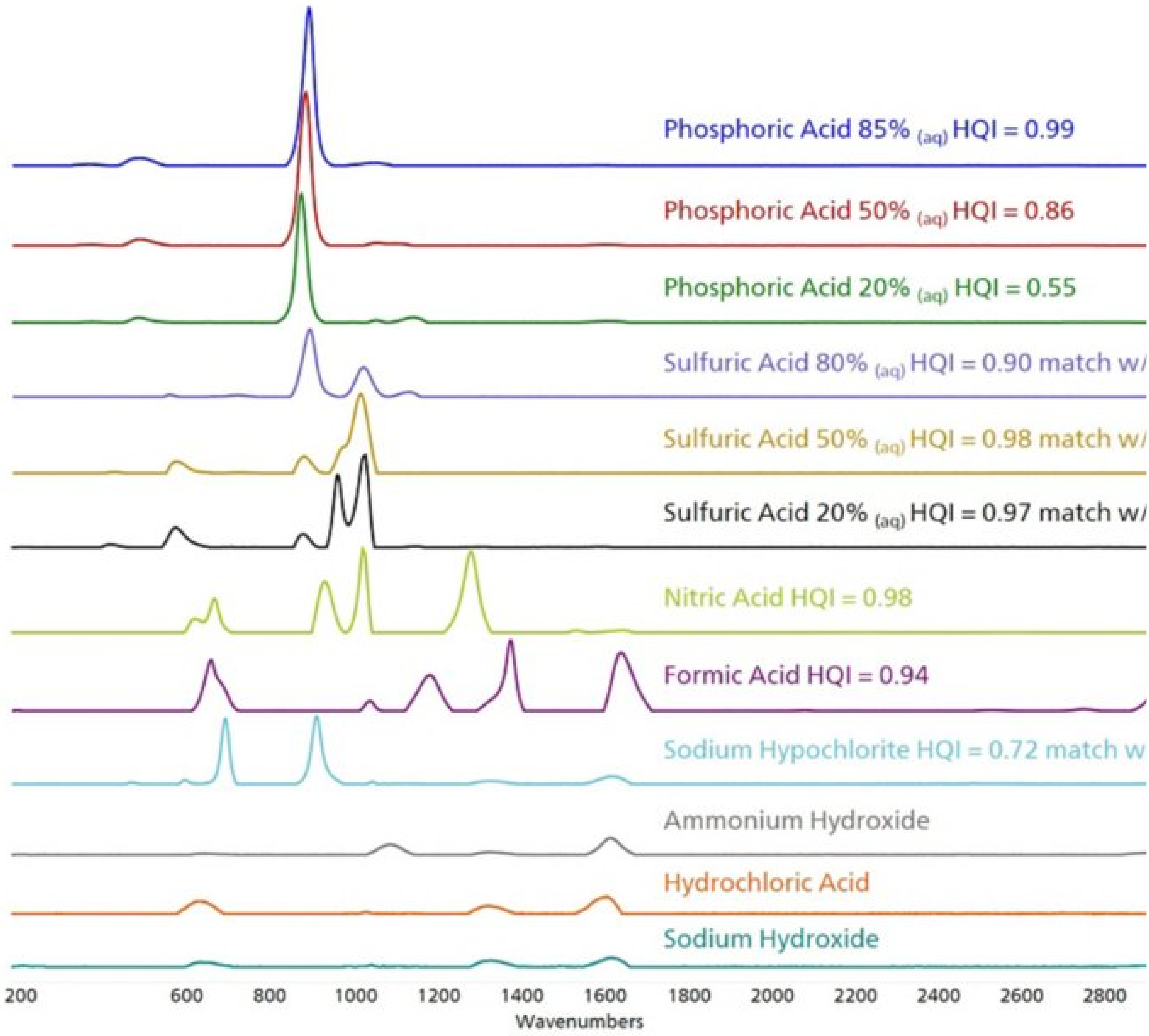

Figure 1. Initial Raman spectra of strong acids and bases.

When possible, Hit Quality Index (HQI) values, which indicate spectral correlation, were included in **Figure 1**. Polyprotic acid dilution reveals the sensitivity of the Raman spectrum to protonation state, both visually and through HQI values. For example, HQI values for dilute phosphoric acid solutions suffer when compared to a library spectrum of concentrated acid, while sulfuric acid (SA) dilutions maintain high HQI values against library spectra of concentrated H_2SO_4.

Of note is the poor Raman response of very small molecules such as hydrochloric acid and sodium hydroxide. Because Raman spectroscopy measures the vibrational energy of molecular bonds, there is very little information in a Raman spectrum of molecules with only ionic and O–H bonds. Such materials cannot be adequately identified through library matching.

Analysis of acids in plastic "lemons"

Phosphoric acid was introduced into a plastic lemon-shaped squeeze bottle and analyzed through the plastic using the Long Working Distance (LWD) attachment (focal length = 8 mm). Sulfuric acid was treated in an identical manner.

Results

A distinct spectrum was acquired for each sample. Comparison of library and experimental spectra confirms peak presence from both the acid and the polyethylene container for each sample (**Figure 2** and **Figure 3**).

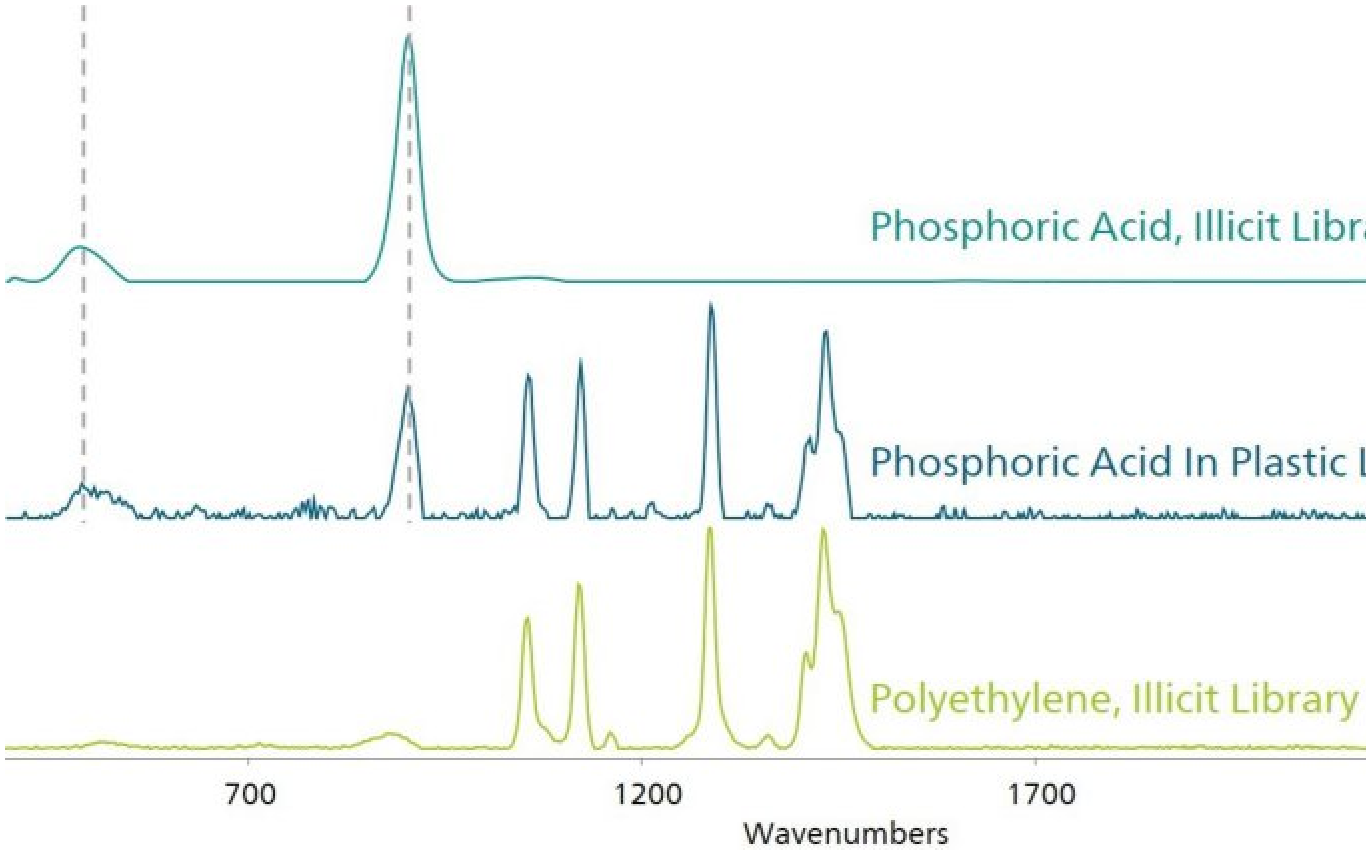

Figure 2. Sample and Illicit library spectra for phosphoric acid.

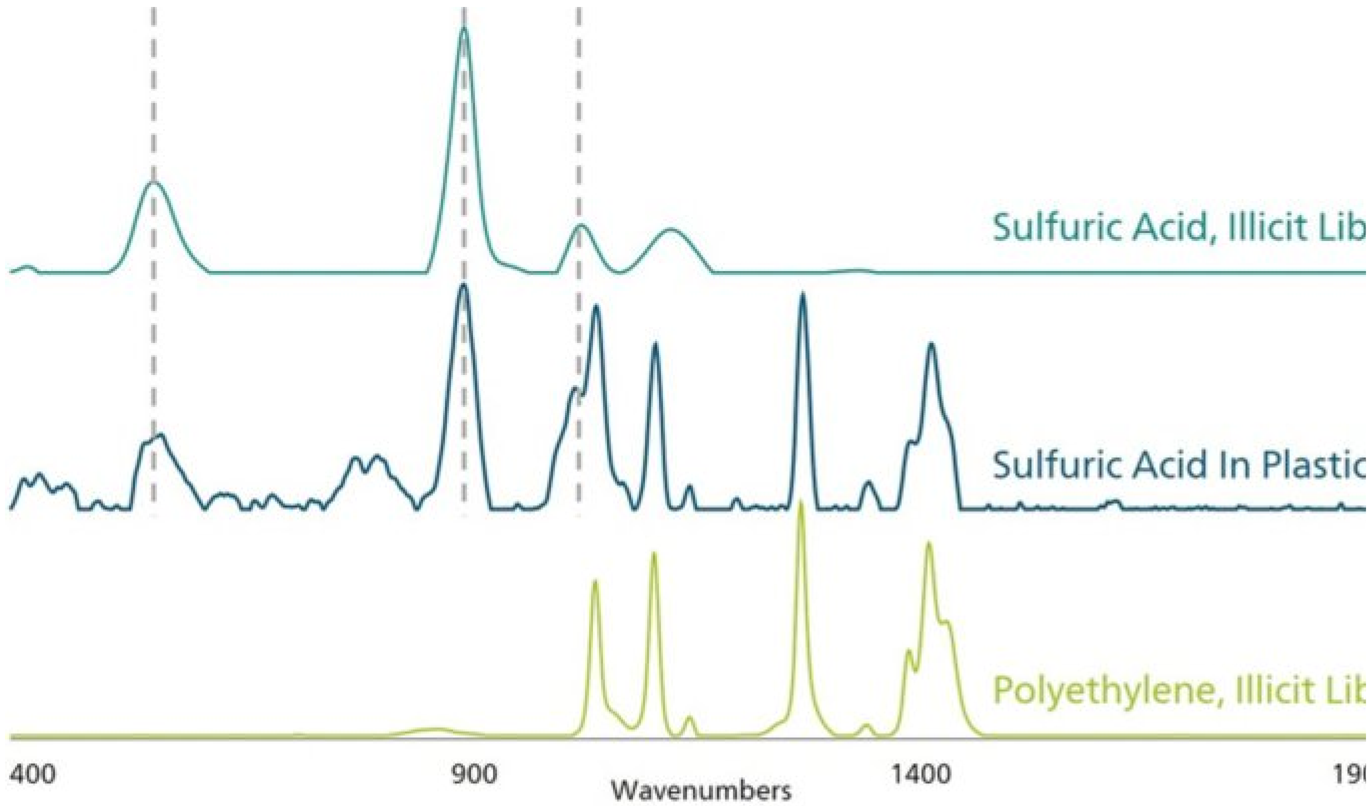

Figure 3. Sample and Illicit library spectra for sulfuric acid.

For the best success in a similar application, MIRA DS users would build Raman libraries containing common, locally available corrosive substances and containers. Custom libraries enable MIRA to provide accurate identification in real-world scenarios.

Conclusion

Modern methods of material identification are required to challenge modern threats. Acid throwing is just one example where MIRA’s small size, fast through-container analysis, and flexible library capabilities enable forensic investigation of suspicious containers. If we can help authorities identify the threat, we can help them prevent damage to society.

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