Application Note AN-RS-012

Handheld Raman for Acid Attack Prevention

Identification of acids through a novel plastic container

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.

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).

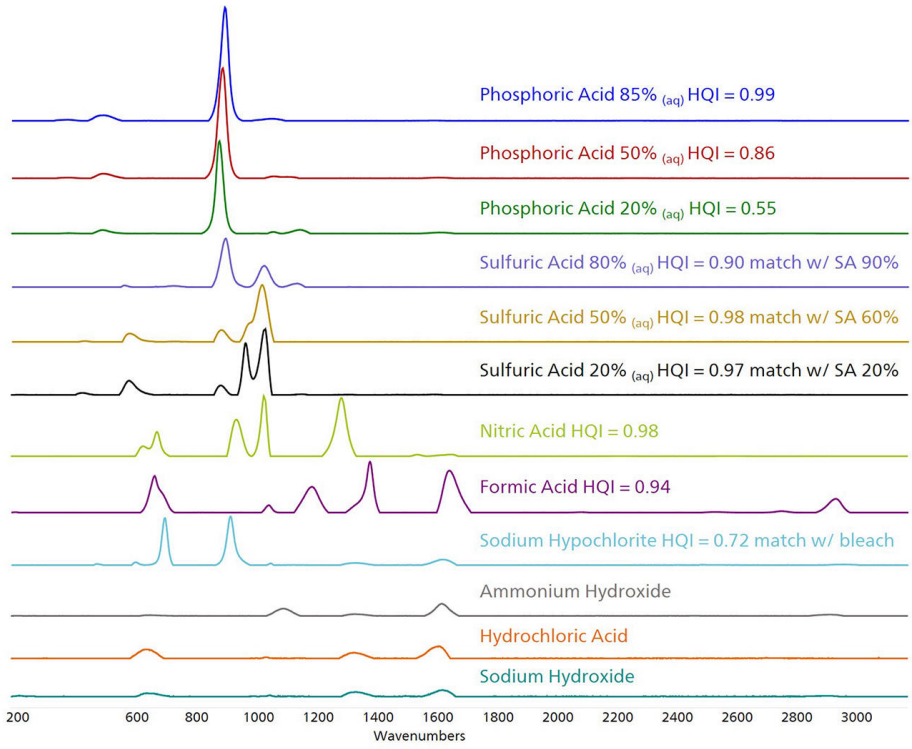

Figure 1. Initial Raman spectra of strong acids and bases.

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).

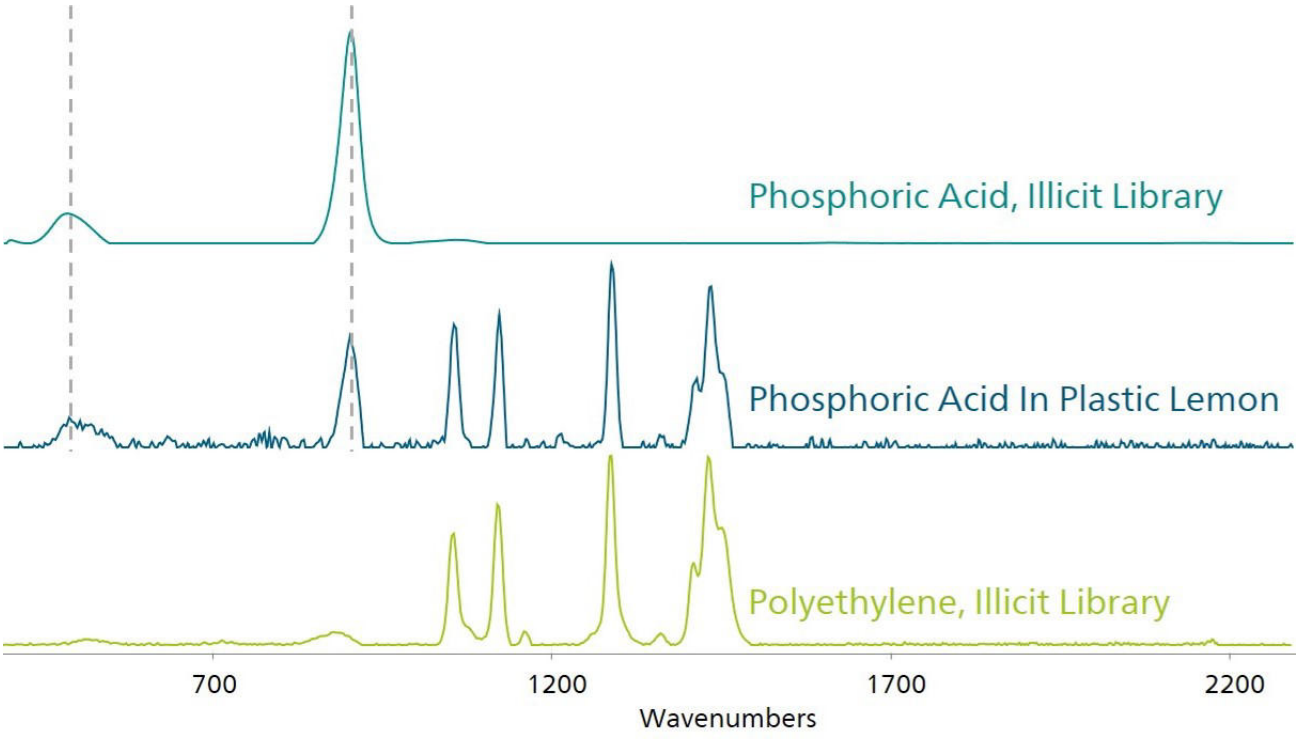

Figure 2. Sample and Illicit library spectra for phosphoric acid.

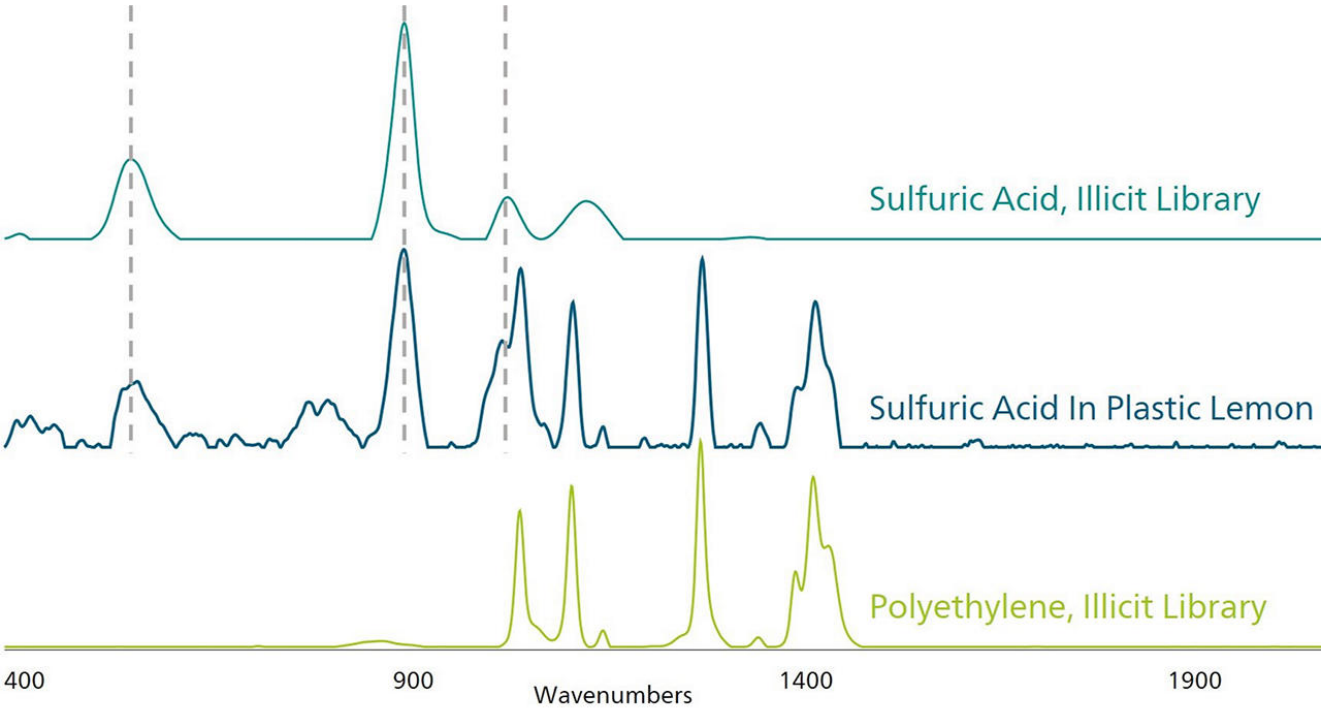

Figure 3. Sample and Illicit library spectra for sulfuric acid.

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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CONFIGURATION

MIRA DS Advanced

Der Metrohm Instant Raman Analyzer (MIRA) DS ist ein robustes, leistungsstarkes Raman-Handspektrometer, das für eine schnelle, zerstörungsfreie Bestimmung verbotener Substanzen, wie z. B. Drogen, Sprengstoffe, Ausgangsstoffe und gefährliche Agenzien, eingesetzt werden kann. Trotz der geringen Grösse ist MIRA DS sehr robust und verfügt über einen hocheffizienten Spektrographen, der mit unserer einzigartigen Orbital-Raster-Scan-Technologie (ORS) ausgestattet ist.

Das Advanced-Paket enthält einen Kalibrierstandard, den Universalaufsatz für Analysen in Flaschen, in Beuteln oder zur direkten Analyse sowie den Winkelaufsatz, der ideal für die Probenanalyse auf einer Oberfläche und/oder in einem Beutel geeignet ist. Betrieb in der Laserklasse 3B. MIRA DS unterstützt Bibliotheken für Raman-Handspektrometer von Metrohm.

Vialhalteraufsatz

Vialhalteraufsatz für Mira M-3/P/DS. Passt zu Glasvials der Grösse 15 x 26 mm.

Aufsatzlinse (LWD)

Im Mira M-3/P/DS Advanced Package ist eine Aufsatzlinse (LWD) für lange Distanz mit einer Brennweite von 7,6 mm enthalten. Betrieb mit Klasse 3B.