



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**).

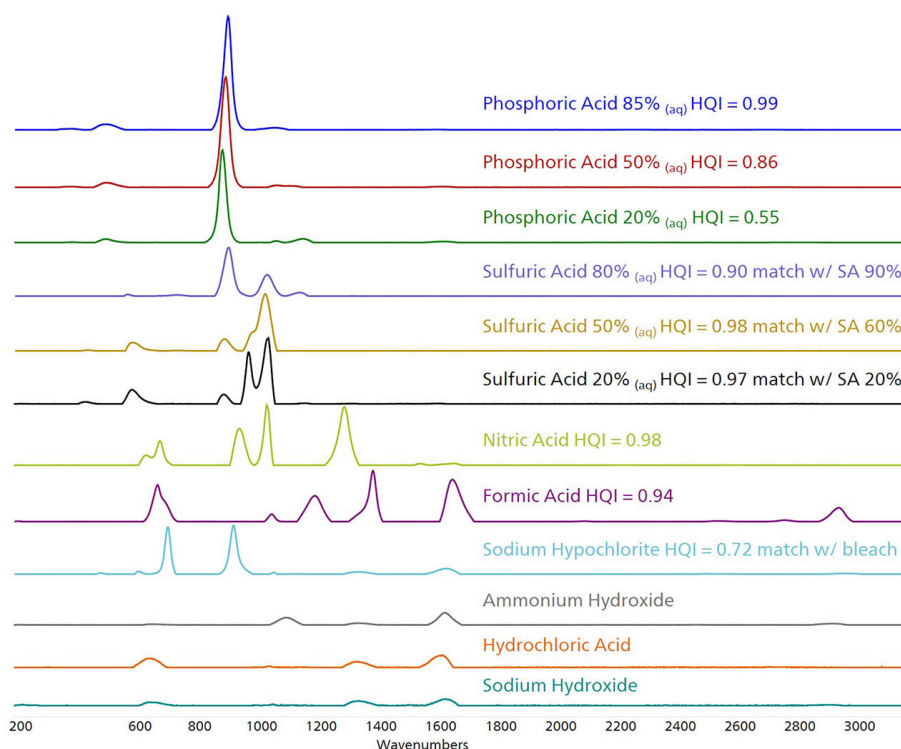


Figure 1. Initial Raman spectra of strong acids and bases.

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).

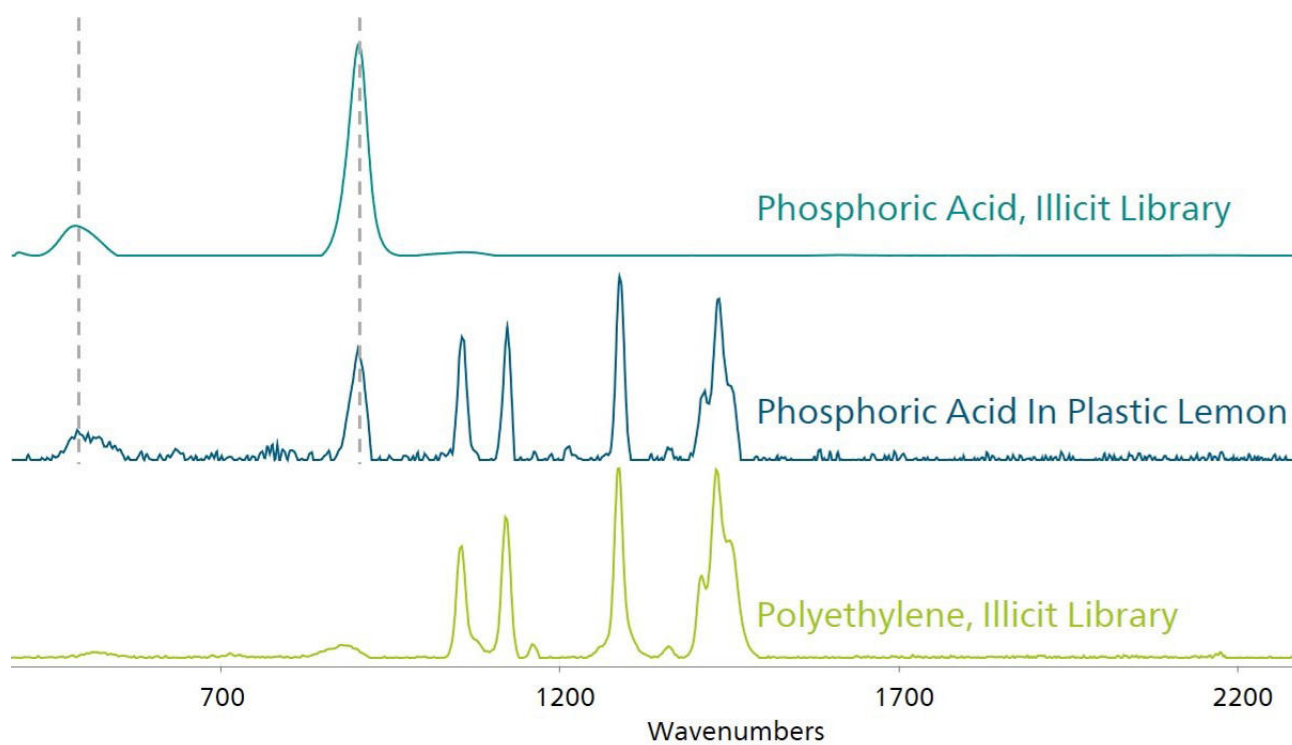


Figure 2. Sample and Illicit library spectra for phosphoric acid.

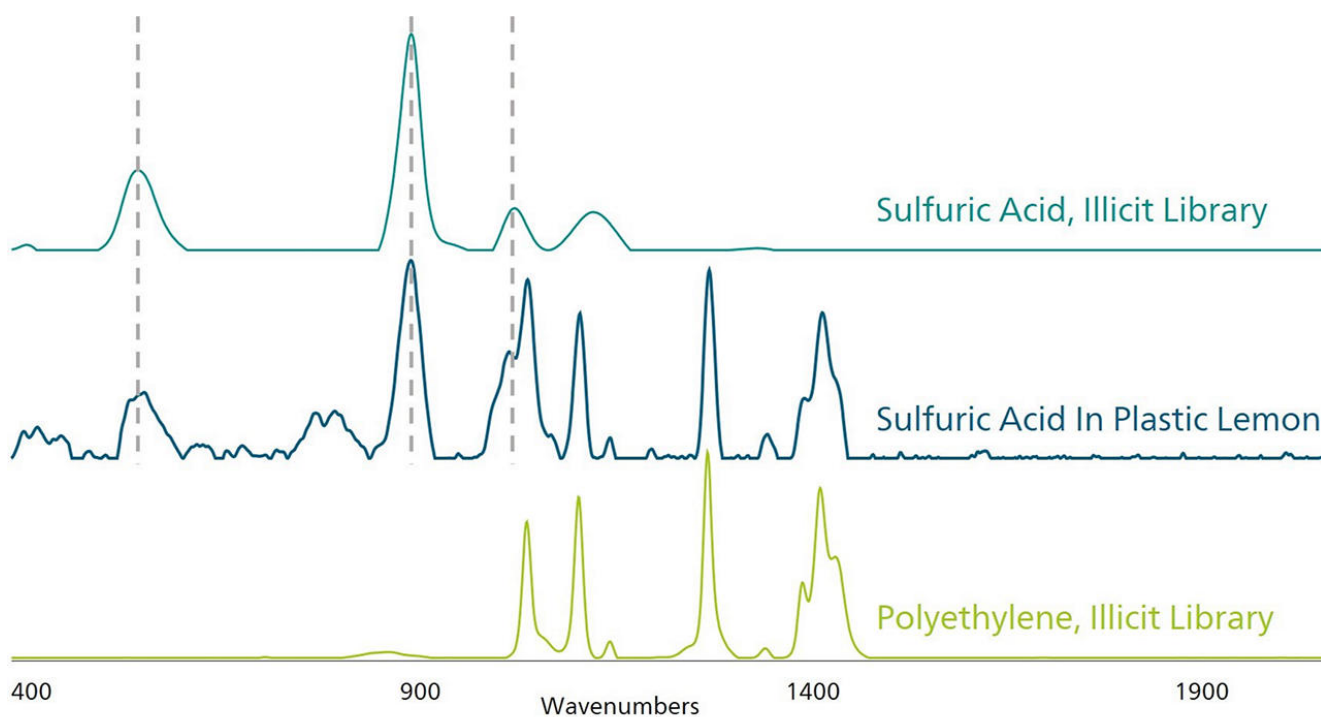


Figure 3. Sample and Illicit library spectra for sulfuric acid.

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.



CONCLUSION



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CONFIGURATION



MIRA DS Advanced

Metrohm Instant Raman Analyzer (MIRA) DS は、薬物、爆発物 出発物質、有害物質などの違法物質の迅速な非破壊測定に使用される、頑丈かつ高性能なハントヘルトラマンスペクトロメーターです。MIRA DS は、小型な装置ながら極めて堅牢で、弊社独自の軌道走査スキャン (ORS) 技術を搭載した高効率分光器を特長としています。

Advanced package には、校正標準、ホトルまたはハックにおける分析または直接分析のためのユニバーサルアタッチメント、直角アタッチメントが含まれ、表面および(または)ハック内でのサンプルの処理に最適です。クラス 3B 操作。MIRA DS は、Metrohm のハントヘルトラマンライフラインに対応しています。



Mira M-3/P/DS 用ハイアルホルターアタッチメント。15 x 26 mmのサイズのカラスハイアルに対応。



LWD

Mira M-3/P/DS Advanced Packageには、焦点距離が7.6 mmの遠距離用アタッチメントレンズ (LWD)が付属しています。クラス3B操作。