# Investigating the Capabilities of Handheld Raman Spectrometers for On-Site Intact Explosives Detection

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## ABSTRACT

This study evaluates the detection capabilities of two handheld Raman spectrometers using analytical standards, such as 2,4,6-trinitrotoluene (TNT), nitromethane (NM), ammonium nitrate (AN), and common smokeless powder components such as diphenylamine (DPA), ethyl centralite (EC), and methyl centralite (MC). Performance metrics assessed included sensitivity, spectral reproducibility, and reliability of internal library matching. An interference study was also conducted using glass and plastic containers. Authentic samples, including TNT flakes, ammonium nitrate/fuel oil (ANFO) mixtures, NM, and disk-shaped smokeless powder, were analyzed to evaluate practical applicability. This work provides practical insight into the performance of handheld Raman devices and offers guidance for their effective deployment.

## INTRODUCTION

In the past few years, law enforcement has been encountering a growing number of civilians in possession of military-grade munitions discarded from conflict zones, alongside a rise in domestically assembled improvised explosive devices (IEDs)[1,2]. Because intact explosives can pose significant risks to investigators, thorough on-site screening of evidence is essential for enhancing their safety by accurately determining the materials present.

The on-site detection of intact explosives poses considerable challenges due to the dangerous and sensitive nature of these materials. Handheld Raman spectrometers have become popular as rapid, non-destructive tools for the identification of unknown materials, as they require no sample preparation.

The explosives analyzed in this study are frequently observed in current forensic casework and have been used in the manufacture of improvised explosive devices (IEDs), including smokeless powder and ANFO.

## MATERIALS & METHODS

**Handheld Raman Spectrometers:** The ResQ-CQL from Rigaku uses a 1064 nm Nd:YAG laser and an adjustable laser excitation power of up to 490 mW (**Figure 1A**), and the HandyRam™ from FieldForensics uses a 785 nm diode laser and a laser excitation power of 100 mW (**Figure 1B**).


**Figure 1:** Images of the two handheld Raman spectrometers.

**Sample Preparation:** Standard solutions were created for TNT, NM, DPA, MC, and EC at concentrations of 1000 mM, 750 mM, 500 mM, 250 mM, 100 mM, and 50 mM in acetone. The same concentrations were created for AN using water as the solvent. Authentic samples of TNT, NM, ANFO, and smokeless powder were also analyzed.

**Measurements:** Seven replicates were collected on each instrument and averaged. Data was collected in the 136–2485 $cm^{-1}$ scan range for the ResQ-CQL and the 400–2300 $cm^{-1}$ scan range for the HandyRam™.

**Metrics Evaluated:** **Sensitivity**- Standard solutions were used to determine the observed limits of detection (LOD) for each analyte, i.e., the lowest concentration where all peaks of interest were present. **Repeatability**- The peak location was recorded for each replicate at each concentration and the average, and 95% confidence interval uncertainty ($\alpha$ = 0.05) was calculated. **Performance of ResQ-CQL internal library** was assessed and an **interference study** using glass and plastic containers was also conducted.

**Data Processing:** Data was analyzed using Microsoft Excel version 16.0 and the optical spectroscopy software Spectragryph.

## RESULTS & DISCUSSION

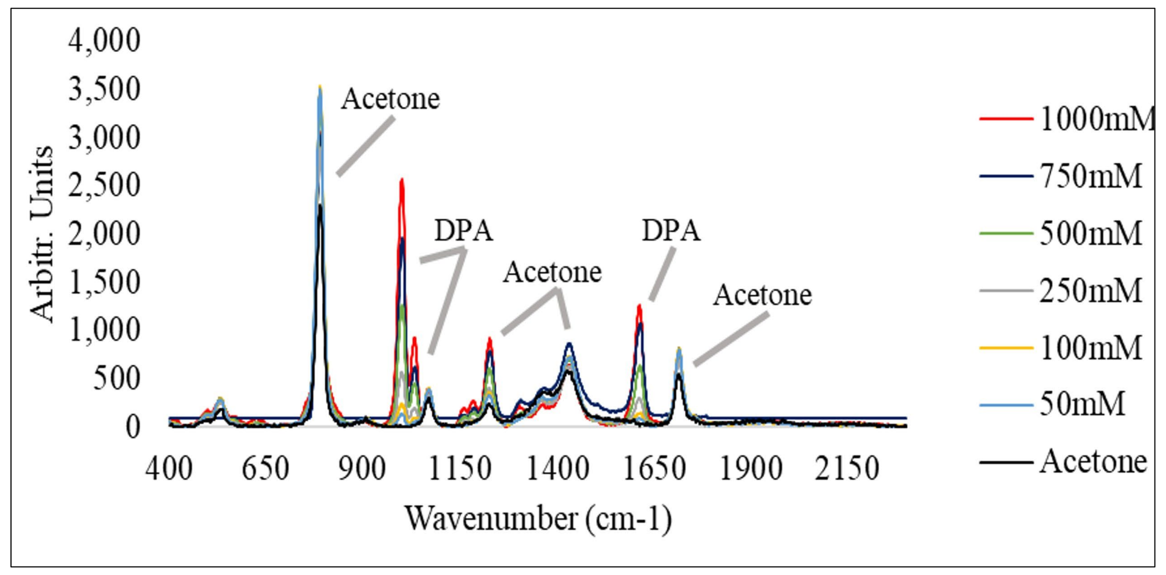


**Figure 2:** Stacked Raman spectra of DPA using the HandyRam™ Raman spectrometer at all studied concentrations.

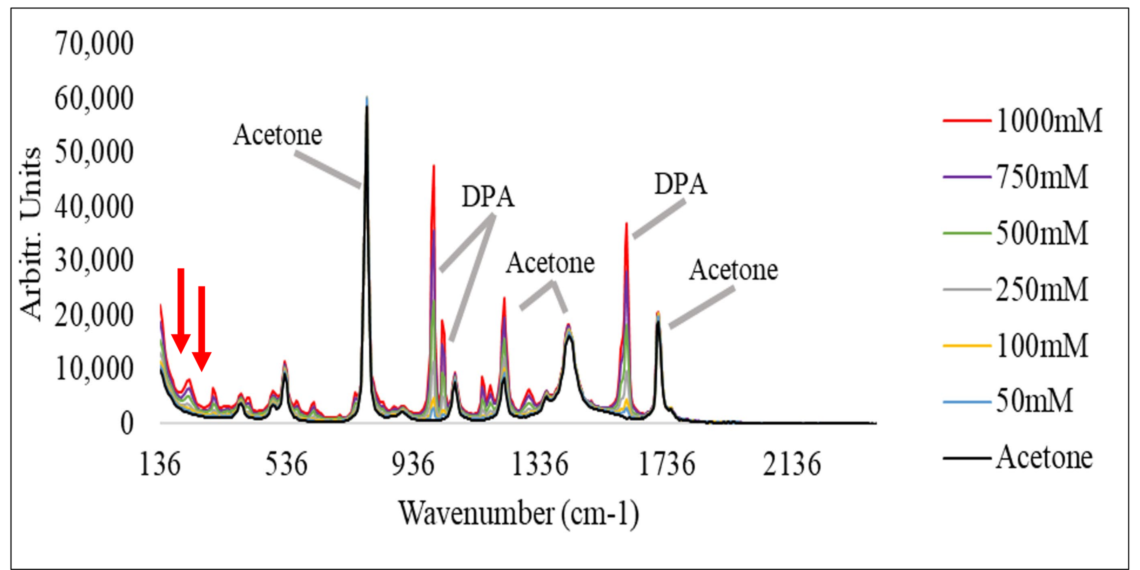


**Figure 3:** Stacked baseline corrected Raman spectra of DPA using the ResQ-CQL Raman spectrometer at all studied concentrations.

**Table 1:** Observed LOD where all the peaks of interest were present for each analyte in both glass and plastic containers using the ResQ-CQL and HandyRam™ portable spectrometers.

| Analyte | ResQ-CQL | | HandyRam™ | |
|---|---|---|---|---|
| | LOD (mM) | | LOD (mM) | |
| | Glass | Plastic | Glass | Plastic |
| TNT | 100 | 100 | 500 | 500 |
| NM | > 1000 | > 1000 | > 1000 | > 1000 |
| DPA | 100 | 100 | 250 | 250 |
| MC | 250 | 250 | 250 | > 250 |
| EC | 250 | 250 | 250 | 500 |
| AN | 50 | 50 | 50 | 250 |

- Spectra showing all characteristic peaks for TNT flakes (**Figure 4A and B**), ANFO, and NM were obtained using both spectrometers.

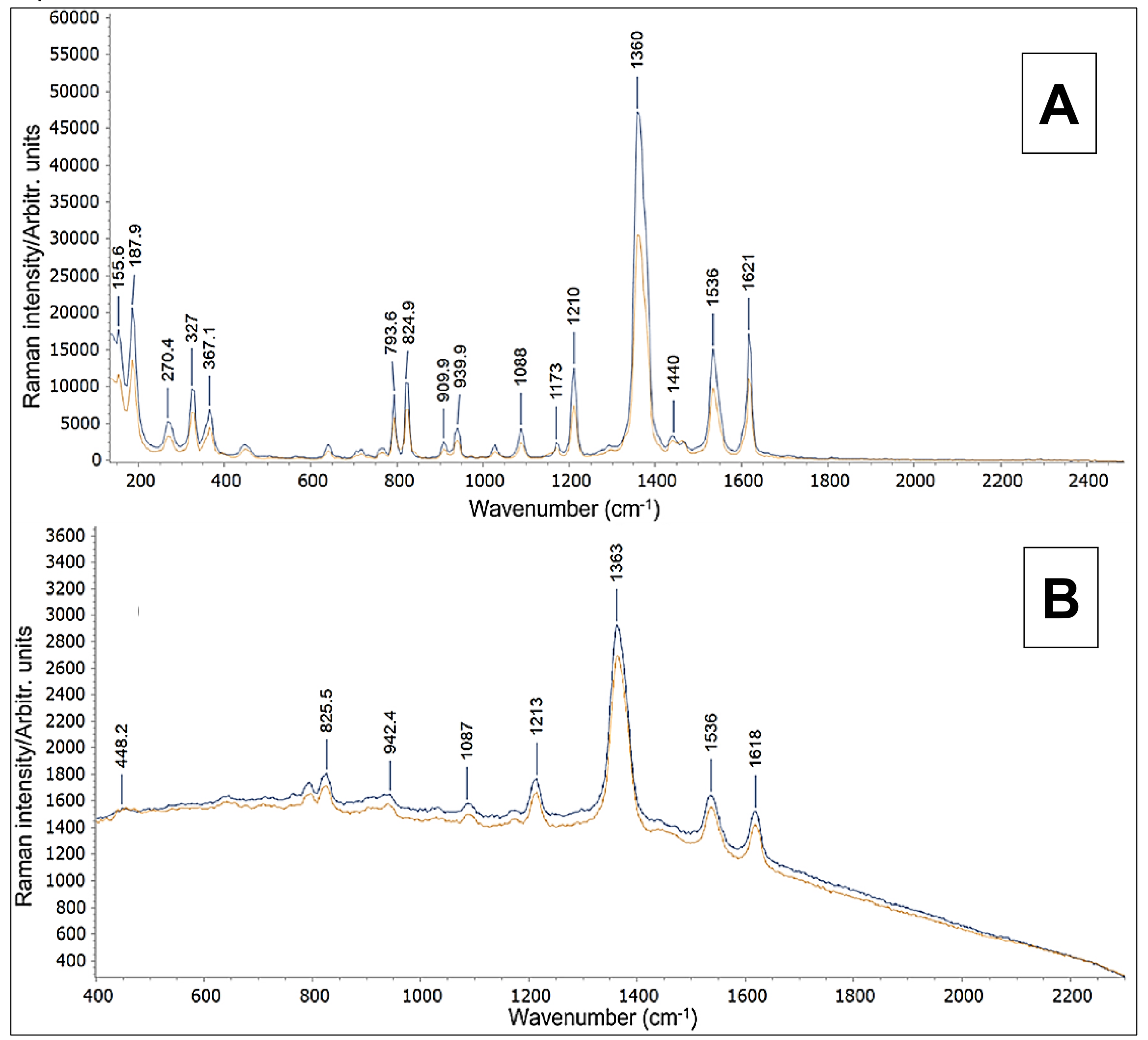


**Figure 4:** Comparison of Raman spectra of authentic TNT flakes using the ResQ-CQL Raman spectrometer **(A)** and the HandyRam™ **(B)** in glass container (blue spectra) and plastic container (orange spectra)

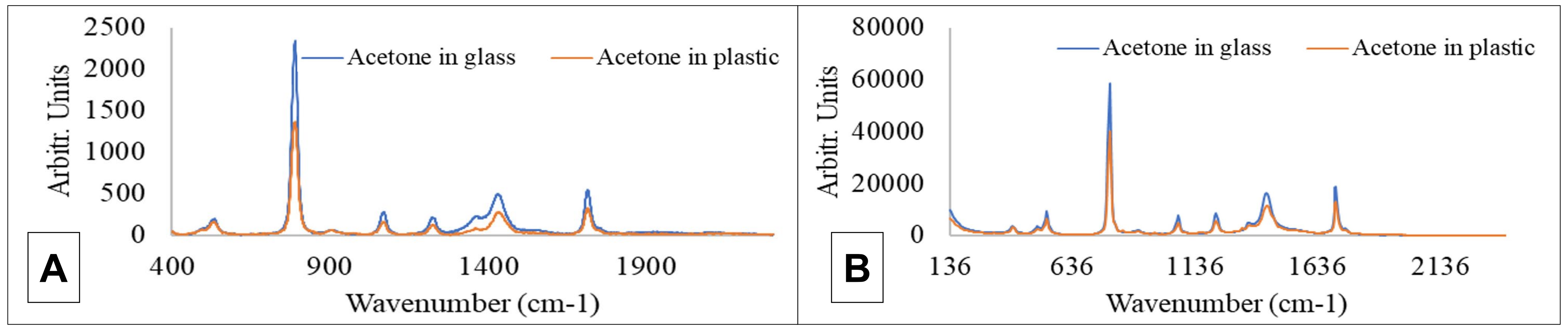


**Figure 5:** Comparison of Raman spectra of acetone collected in a glass container (in blue) and a plastic container (in orange) using the HandyRam™ **(A)** and Rigaku ResQ-CQL **(B)**.

- Using the HandyRam™, the band located around 1400 $cm^{-1}$ in **Figure 5A** exhibits a slight broadening, which could indicate that the glass is causing minor spectral interference with the spectrum of acetone.
- A decrease in signal was observed for the data collected from the plastic container using both handheld spectrometers (**Figure 5A and 5B**).

- Both spectrometers produced reproducible spectra with consistent peak positions and intensities across all standard analytes.
- As shown in **Figures 2 and 3**, the spectra collected with the HandyRam™ were observed to be much less intense than that of the ResQ-CQL.
- The ability to obtain data below 400 $cm^{-1}$ with the ResQ-CQL proved to be extremely beneficial, especially for DPA.
- Two additional peaks, located at 226 $cm^{-1}$ and 303 $cm^{-1}$ (indicated by red arrows in **Figure 3**), were identified as being characteristic of DPA.
- Of the "misidentified" analytes (in red in **Table 2**), most were not technically misidentified. The spectrometer identified the solvent instead of the explosive due to limitations with LOD (**Table 1**).
- The library in the ResQ-CQL correctly identified AN down to 100 mM in glass and 250 mM in plastic (**Table 2**).
- This could be due to the lack of solvent peak interference, compared to other analytes.

**Table 2:** Percentage of correctly identified analytes in glass and plastic using Rigaku ResQ-CQL's internal library.

| | | | Percentage of correctly identified analytes (%) | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | *Pure solid/liquid* | *1000 mM* | *750 mM* | *500 mM* | *250 mM* | *100 mM* | *50 mM* |
| Analyte | *AN* | Glass | 100 | 100 | 100 | 100 | 100 | 100 | 43 |
| | | Plastic | 100 | 100 | 100 | 100 | 100 | 0 | 0 |
| | *DPA* | Glass | 100 | 100 | 0 | 0 | 0 | 0 | 0 |
| | | Plastic | 100 | 0 | 0 | 0 | 0 | 0 | 0 |
| | *EC* | Glass | 100 | 0 | 0 | 0 | 0 | 0 | 0 |
| | | Plastic | 100 | 0 | 0 | 0 | 0 | 0 | 0 |
| | *MC* | Glass | 100 | 0 | 0 | 0 | 0 | 0 | 0 |
| | | Plastic | 100 | 0 | 0 | 0 | 0 | 0 | 0 |
| | *NM* | Glass | 100 | 0 | 0 | 0 | 0 | 0 | 0 |
| | | Plastic | 100 | 0 | 0 | 0 | 0 | 0 | 0 |
| | *TNT* | Glass | 100 | 100 | 57 | 100 | 0 | 0 | 0 |
| | | Plastic | 100 | 100 | 57 | 100 | 0 | 0 | 0 |

## CONCLUSIONS

- The ResQ-CQL1064 nm laser and higher laser power allowed for the best balance between low background fluorescence and high signal of the analyte of interest.
- The HandyRam™ used in this study was manufactured in 2015 and has since been replaced by the HandyRam™ II.
- The HandyRam™ II is equipped with Rapid Laser Spin (RLS™) technology, which uses rastering, and decreases the risk of thermally degrading samples or detonating energetic materials, as well as improving spectral quality for heterogeneous or complex samples.

## ACKNOWLEDGEMENTS

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## REFERENCES

[1] United States Bomb Data Center, United States Bomb Data Center (USBDC) Explosives Incident Report (EIR) 2023, Bureau of Alcohol, Tobacco, Firearms, and Explosives.

[2] D. J. Klapec et al., Interpol review of the analysis and detection of explosives and explosive residues. Forensic Science International: Synergy. Volume 6, 2023, 100298. https://doi.org/10.1016/j.fsisyn.2022.100298

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