The Impact of Glass Vial Type in Measuring Raman Spectrum of Liquid Hydrocarbon Samples

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INTRODUCTION

Raman spectroscopy has been increasingly used in forensic science over the recent decades due to its myriad of benefits. This method has been developed to become relatively inexpensive, rapid, nondestructive, and accepted by the scientific community, making it valuable in forensic chemical identification and classification. It also has confirmatory potential when paired with multivariate statistical methods, even when it is a portable instrument [1]. However, further use of Raman spectroscopy has been found to have difficulties with vial types. Vials labeled as the same composition of glass can lead to varying results for the same sample with this spectroscopic method. The varying results obtained from the same sample may be due to the composition of glass vials producing interfering fluorescence in the spectra [2].

Thus far, research on the relationship between fluorescence and Raman spectroscopy with reference to sample vials is limited. Several methods are available to overcome the obstacle of fluorescence in Raman spectroscopy. These methods include Shifted Excitation Raman Difference Spectroscopy (SERDS), adjusting laser excitation wavelength, and computational methods in postprocessing [3]. When these methods are not implemented, the detection of Raman scattering signals may be adversely impacted by the composition of the vials used to conduct experiments. By applying a protocol that detects the interference of vials, laboratories can limit the room for error and consequently save time and money.

MATERIALS & METHODS

In this work, the following materials were used:

- Handheld Raman spectrometer (HandyRam)
- 10 mm standard rectangular cell Quartz cuvette
- Amber Type 1 Borosilicate vial (B75562)
- Clear Vial Black Foam Lined Cap (V1526C-FM)
- Clear Vial PTFE Lined Cap (V1526C-TFE)
- Standard neat jet fuel

RESULTS & DISCUSSION

- In Figures 1 and 2, the background signal of the B75562 vial appears similar to that of the quartz cuvette.
- As a result, the spectra of the quartz cuvette and B75562 vial containing the standard neat jet fuel sample displayed a better quality of Raman spectra, as seen in Figures 1 and 2, respectively.

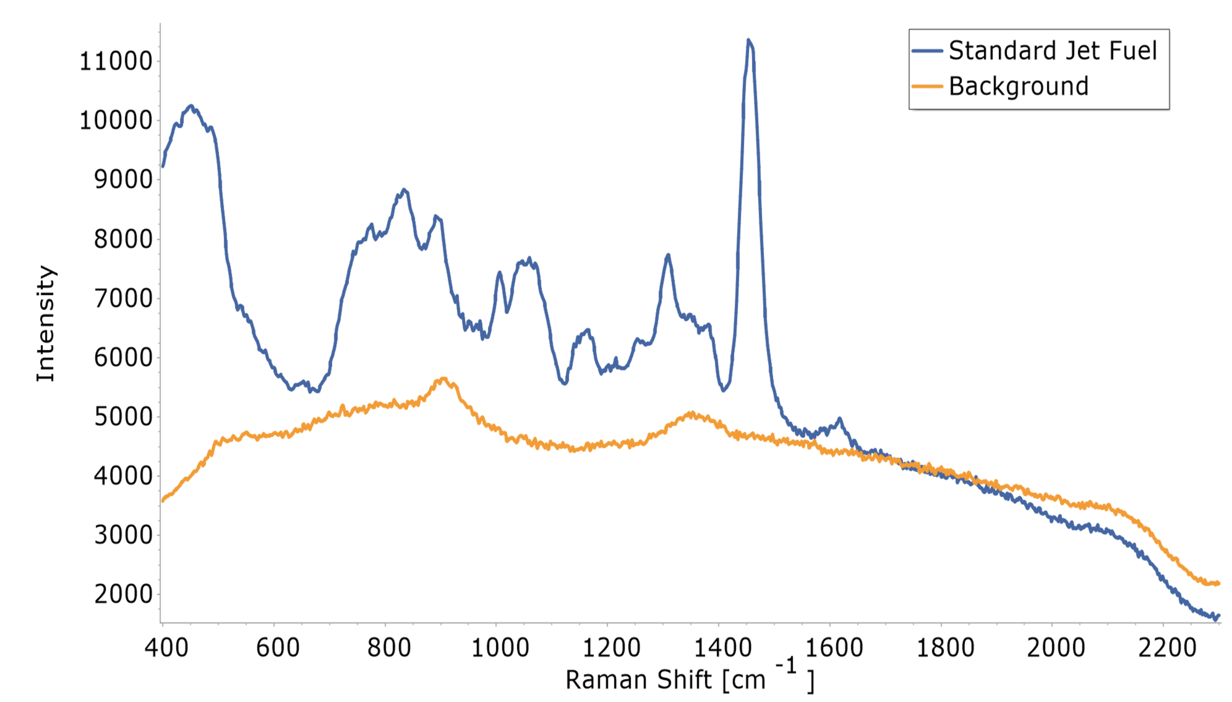

Figure 1. Quartz cuvette background and standard jet fuel spectra.

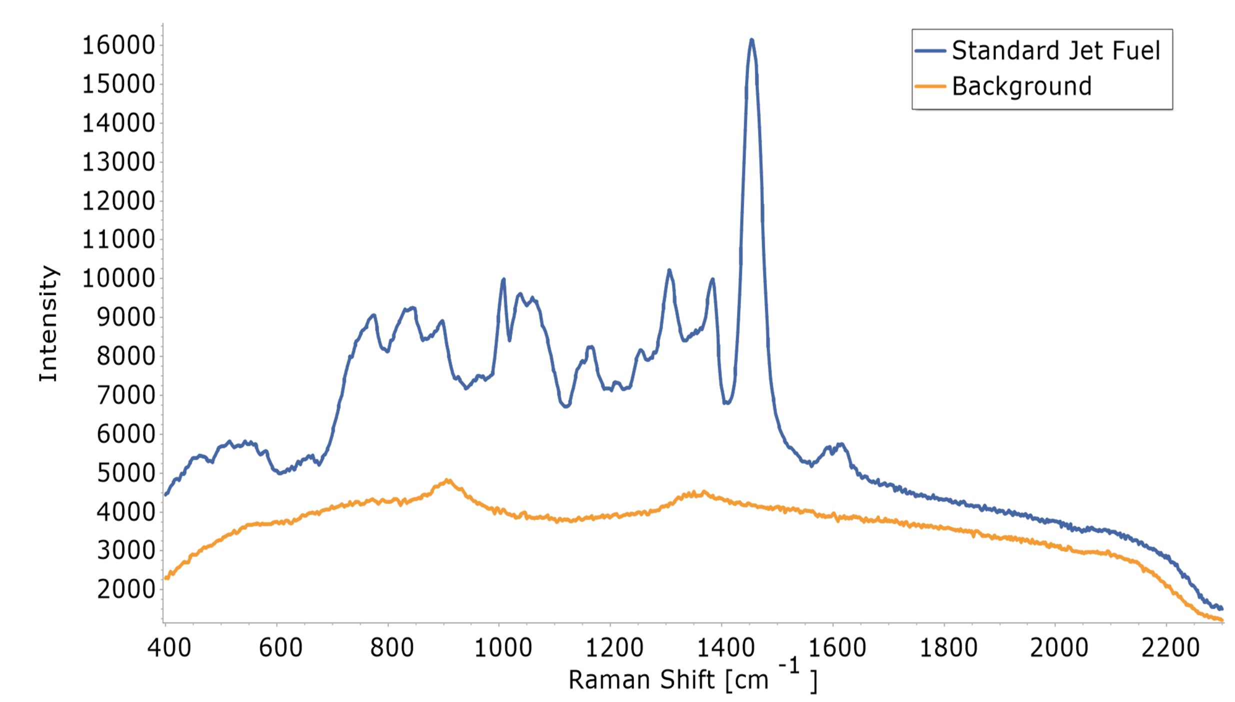

Figure 2. Amber Type 1 Borosilicate Vial (B75562) background and standard jet fuel spectra.

- Although the V1526C-FM and V1526C-TFE vials are made of borosilicate, they produce a large background peak at ~1384 cm^{-1} in the spectra, as seen in Figure 3 and 4 respectively, leading to inconclusive results for liquid hydrocarbon samples. This illustrates the importance of collecting background spectra of sample containers before sample testing to guarantee adequate quality of Raman spectra.
- The background signals produced from the V1526C-FM and V1526-TFE vials, in Figure 3 and 4 respectively, could be detected and noted as problematic by taking the background spectra of the vials.

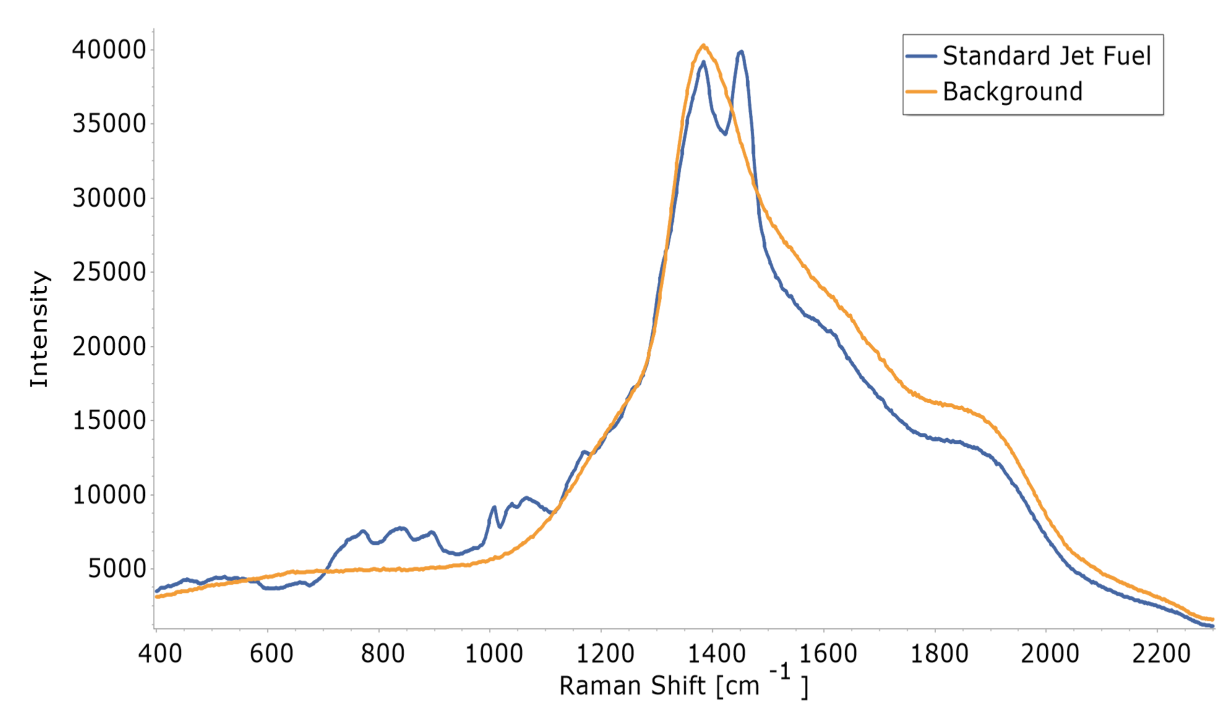

Figure 3. Clear Vial Black Foam Lined Cap (V1526C-FM) background and standard jet fuel spectra.

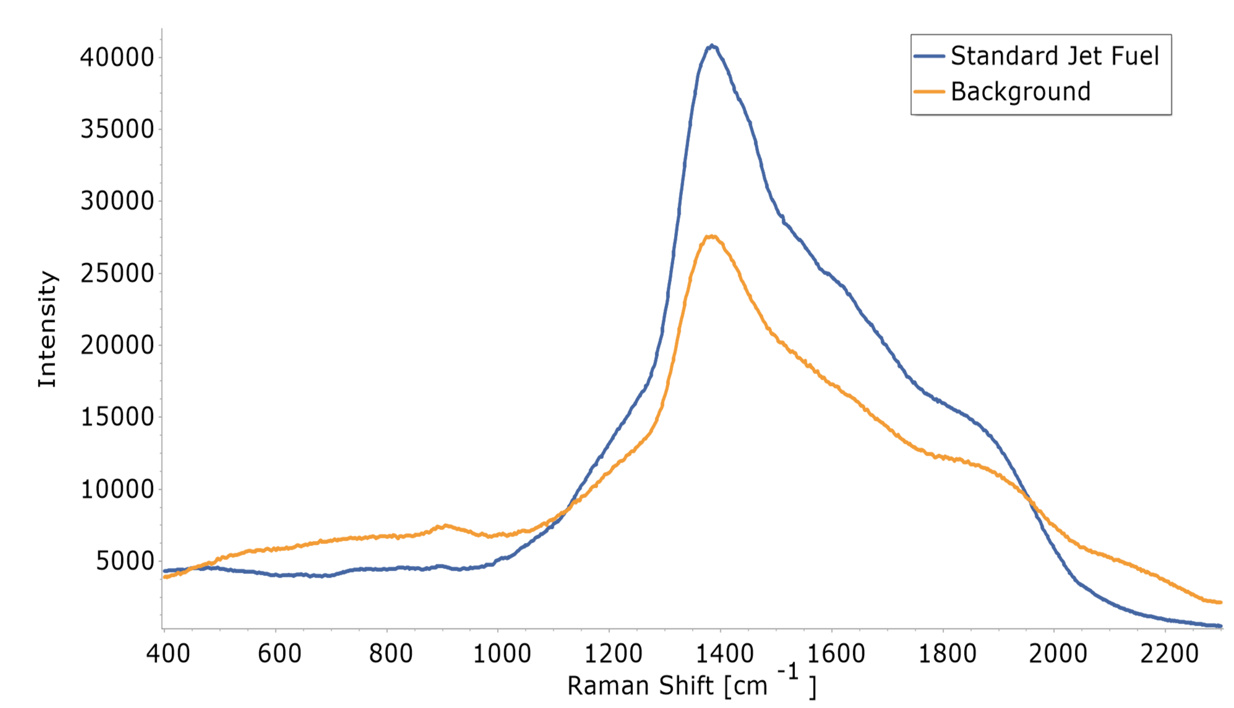

Figure 4. Clear Vial PTFE Lined Cap (V1526C-TFE) background and standard jet fuel spectra.

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MATERIALS & METHODS

The handheld Raman spectrometer (HandyRam, Field Forensic Inc., St. Petersburg, FL, USA) point-and-shoot method was used to obtain each container's spectra in two different instances. In one instance, each container held 2 mL of standard neat jet fuel sample, while the other spectra were obtained with no sample in the vial. Raman scattering signals were collected using autointegration with raster mode enabled and a laser power set to 1, with no post-measurement data treatment applied to the spectra. Three replicate Raman spectra were collected from three vials of each type in both instances. All Raman spectra were acquired with a 785 nm laser and recorded a spectral range of 400 – 2300 cm^{-1} at 1 cm^{-1} intervals. All spectral data acquisition was performed using Peak software (V1.01.0068, Snowy Range Instruments, Wyoming, USA). Figures 1 – 4 were created using the Spectragryph 1.2 software.

CONCLUSIONS

In summary, since glass vials are not specifically made or marked for Raman spectroscopic techniques, it is crucial to collect a background spectrum of the sample container prior to sample testing. This study demonstrates the critical role of the vial glass type in collecting acceptable Raman spectra for liquid hydrocarbon samples. This work proposes a testing protocol to ensure high-quality spectra are collected, and the results include an awareness of the importance of vial composition when using Raman spectroscopy.

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