Smartphone Operated Handheld Raman Spectrometer for Explosives Detection/Identification: A portable tool for First Responders

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Abstract

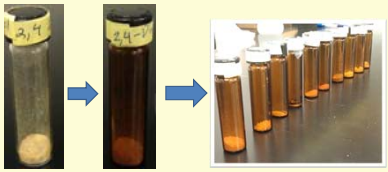
A Raman spectral library for Agiltron's PinPointer™ system, a portable handheld Raman spectrometer operated by commercial Smartphones and Palm PCs is being developed for in-field detection of explosives and threat chemicals. The PinPointer™ spectrometer uses a 785 nm excitation wavelength with adjustable power from 5 to 300 mW and covers the 200-3000 cm^{-1} Raman shift spectral range. The hand-held portable spectroscopic system runs on a rechargeable battery. The targets for spectral acquisition were crystalline solids, powders and hazardous liquids, including precursors of highly energetic materials (HEM) from the list of explosive materials published in the Bureau of Alcohol, Tobacco, Firearms and Explosives (BATF). Powders and liquids were tested through either clear or amber vials while crystals were tested through direct contact with the laser lens. With special attention to fluorescence minimization by recrystallization and laser output optimization as a criteria, a total of 59 chemicals have been added to the library of hazardous materials (HazMats) and explosives. A subset of 10 chemicals already added to the library was positively identified in amber vials at select laser outputs with hit quality indices greater than 90%. Of the 12 fluorescent substances that were recrystallized, 8 demonstrated endogenous fluorescence, 3 demonstrated exogenous fluorescence and one remained unclassifiable because of its highly absorbing nature at the laser wavelength. Future work includes continuing spectral acquisition of threat chemicals as they become available and testing their detectability in other containers and on flat surfaces, such as glass, aluminum and stainless steel.

Relevance

Rapid, precise explosives identification is one of the central tasks of homeland security and public safety personnel, particularly with the recent proliferation of improvised explosive devices (IEDs) worldwide. Instruments that can be used in the field to rapidly and accurately identify various explosives and their precursors are integral tools for first responders. Handheld instruments employing Raman spectroscopy have recently become powerful tools for on-scene analyses of unknown materials. Raman spectroscopy is particularly well suited for the field analysis of hazardous materials not only because it produces real-time results, but because it may be used without sample preparation or contact. In fact, the laser-based method can be performed through transparent containers such as glass or plastics, significantly reducing the potential of chemical hazards to the investigator as well as contamination of forensic evidence.

Technical Approach

Detectability in Amber Vials



Spectra of 59 threat chemicals were saved onto the developing library, all of which either derived from clear vials or direct contact with laser lens. A subset of 10 chemicals were positively identified in amber vials at select laser powers with HQI's > 90%.

Chemical	Laser Output, mW	Hit Quality Index (HQI)
p-Nitroaniline	5	98.3 %
p-Nitroaniline	300	98.4 %
4-Nitrobiphenyl	5	97.8 %
4-Nitrobiphenyl	300	99.2 %
3,4-Dinitrotoluene	50	98.3 %
3,4-Dinitrotoluene	200	98.3 %
3-Nitro-o-xylene	5	94.5 %
3-Nitro-o-xylene	300	92.4 %
4,4-Dinitrobiphenyl	5	99.5 %
4,4-Dinitrobiphenyl	300	99.2 %
p-Dinitrobenzene	5	98.0 %
p-Dinitrobenzene	300	98.8 %
o-Nitrobenzylchloride	100	94.2 %
o-Nitrobenzylchloride	200	97.1 %
2,4-Dinitrophenol	5	96.3 % Multiple Match (1)
2,4-Dinitrophenol	300	98.5 % Multiple Match (1)
n-Methyl-p-nitroaniline	5	99.3 %
n-Methyl-p-nitroaniline	300	97.5 %
2-Methyl-5-Nitrophenylisocyanate	50	98.3 %, Multiple Match (2)
2-Methyl-5-Nitrophenylisocyanate	300	98.8 %

Fluorescence by Impurities

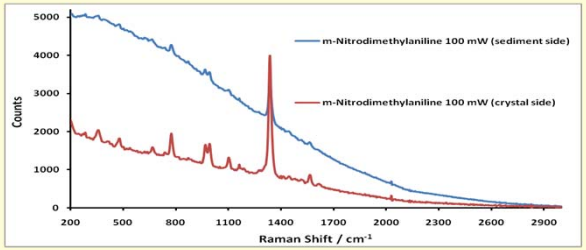


Figure 1: The fluorescence effect of impurities on a sample was observed for m-nitrodimethylaniline at 100 mW upon turning the vial to a spot with more sediment.

Recrystallizations

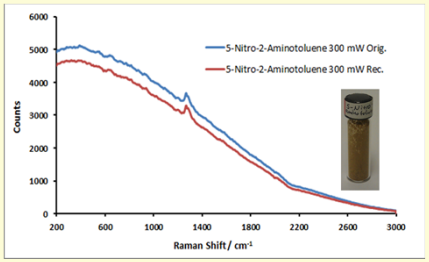


Figure 2: Raman spectra of recrystallized and non-recrystallized forms of 5-nitro-2-aminotoluene at 300 mW. .

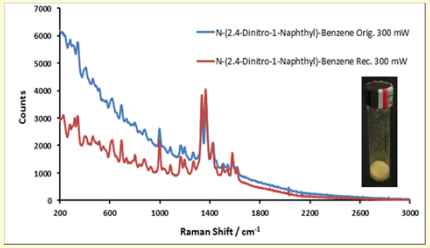


Figure 3: Raman spectra of recrystallized and non-recrystallized forms of N-(2,4-dinitro-1-naphthyl)-benzene at 300 mW.

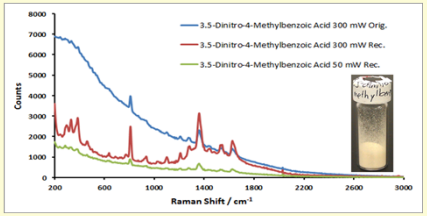


Figure 4: Raman spectra of recrystallized and non-recrystallized forms of 3,5-dinitro-4-methylbenzoic acid at 300 mW and 50 mW.

Future Work

- Continuing to build spectral library as threat chemicals become available.
- *Testing detectability of threat chemicals on flat surfaces such as glass, aluminum and stainless steel and establishing limits of detection.*
- *Testing detectability of threat chemical mixtures in solution.*

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S.P. Hernández-Rivera, J.R. Castro-Suarez, L.C. Pacheco-Londoño, O.M. Primera-Pedrozo, N. Rey-Villamizar, M. Vélez-Reyes and M. Diem, "MID-Infrared Vibrational Spectroscopy Standoff Detection of Highly Energetic Materials: New Developments", *Spectroscopy*, Defense and Homeland Security Issue, April, 2011, 34-41.

Other References

For more information, please go to:
http://academic.uprm.edu/ccsde/

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