Detection and Discrimination of Explosives and Explosive Mixtures by Remote Raman Spectroscopy

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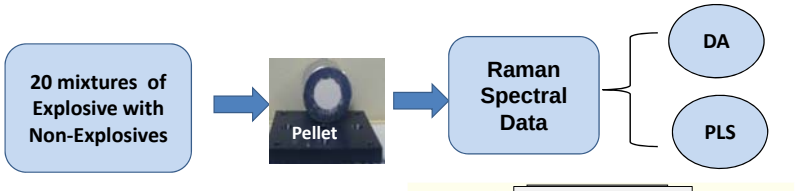
Abstract

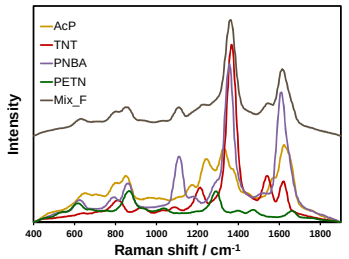
Remote Raman detection has become a powerful analytical technique for detection of hazardous compounds *in situ* and without sample preparation at distances away from the observation site. We report on our efforts in the design, assembly and testing of Remote Raman systems intended for standoff detection of high explosives, such as TNT, DNT, PETN, RDX and HMX and homemade explosives: HMTD, TATP. These energetic compounds have been detected at remote distance employing 532 nm excitation lines from pulsed Nd:YAG laser (5 ns pulses at 10 Hz). Detection limit measurements were carried out for the above mentioned explosives obtaining LOD values below 150 µg using the second harmonic of a pulsed Nd:YAG laser as excitation source. Chemometrics studies, such as partial least squares regressions coupled to discriminant analysis (PLS-DA) were developed for mixtures of explosives with pharmaceutical compounds. The PLS-DA models were applied to the quantification and discrimination of the samples as "explosive" or "non-explosive".

Relevance

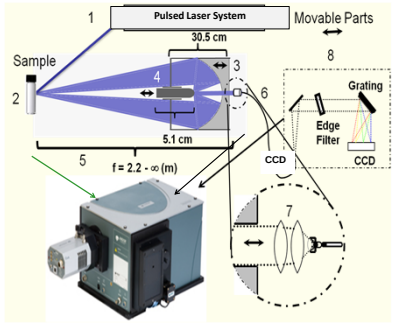
Using a well designed Raman detection system, vibrational signatures of hazardous compounds: HEM/HME can to be recorded at target distances of several meters to hundreds of meters. Raman detection allows for real time analysis, without sample preparation, no human contact, solventless and complementary results can be obtained, allowing for sensor fusion applications. Possible damage caused by terrorist action, in the case that the HEM is detonated can be minimized by remote detection of HEM.HME, CHEMBIO threats and others.

Technical Approach

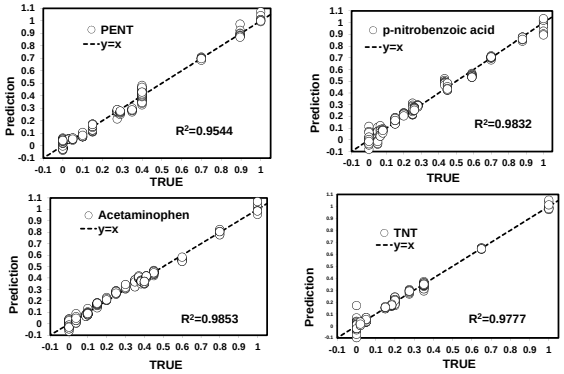




Remote Raman spectra of explosives and non-explosives compound employed in this study



Remote Raman system set-up for explosives detection.



PLS plots for the individual component explosives and non-explosives in different mixtures.

	PNBA	PETN	TNT	Acetaminophen
Spectral region (cm^{-1})	1756-1623	1223-1087	1756-1220	1359-1220
		960-823	1090-957	1090-957
			826-421	826-421
Preprocessing	MSC	SVN	First derv + MSC	MSC
R2	98.82	98.82	99.48	99.21
R2CV	98.41	98.69	98.95	0.0248
RMSEE	0.034	0.030	0.018	0.023
RMSECV	0.030	0.031	0.024	0.030
RMSEP	0.027	0.028	0.045	0.030
Rank	8	7	10	9
LOD (mg)	0.090	0.10	0.15	0.10

PLS summary for Detection of explosives and non-explosives employing 532 nm excitation line, 300 pulses at 10 m

	Pre processing	TP	TN	FP	FN	Sensitivity	Specificity
PNBA	MSC	18	8	3	7	0.7	0.7
PETN	SVN	16	11	2	7	0.7	0.8
TNT	First derv + MSC	16	12	1	7	0.7	0.9
Acetaminophen	MSC	21	7	0	7	0.8	1.0

PLSDA summary results for detection of explosives and non-explosives.

Accomplishments Through Current Year

- Design and development of remote Raman spectroscopy detection system
- Remote Raman detection of CWAS and TICS concealed at different commercial bottles.
- Remote Raman detection of HEMs at very long ranges (> 140 m). Bulk detection of AN.
- TNT Detection samples 2 mm in diam. at 60 m range.
- Discrimination and quantification studies: of explosives and mixtures of explosives with non-explosives compounds

Future Work

- Carry out standoff UV vapor detection of homemade explosives.
- Carry out standoff detection of alkaloid compounds for as possible interferences.

Opportunities for Transition

Defense and Security agencies as well as private sector are highly interested in finding new ways of detecting HEM/HME, hazardous chemicals TIC, TIM and microorganisms.

- ➢ Food industries
- ➢ Environmental Protection Agencies
- ➢ Pharmaceutical Industries
- ➢ Drug Enforcement Administration
- ➢ Biotechnology Industries
- ➢ Petrochemicals industries
- ➢ Other industries

will also benefit from remote detection measurements

Publications Acknowledging DHS Support

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Other References

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

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