Fourier transform infrared (FTIR) spectroscopy has gained significant attention among the forensic scientists because it shows high sensitivity and selectivity, and offers near-real-time detection. Application of the multivariate statistical techniques for the analysis of the spectra is necessary in order to enable feature extraction, proper evaluation and identification of obtained spectra. In this paper we show the development of a feasible procedure for the characterization of spectroscopic signatures of the explosive materials in the remnants after explosion. In our research especially designed and prepared sample catchers were used during the blasts of three various high explosives: C-4, TNT and PETN. Principal component analysis (PCA) was performed using broad spectral data range (600–4000 cm\(^{-1}\)) for sample classification into separate classes. Most of the information contained in spectral data was compressed by PCA in few relevant principal components that explain most of the variance of spectral data. The results show that FTIR spectroscopy in combination with multivariate methods are well suited for identification and differentiation purposes even in very large data sets and could be employed by forensic laboratories for rapid screening analysis.

1. Materials and methods

Small amounts (<30 g) of C-4 (plastic explosive in which the main component is the high energetic material RDX – cyclotrimethylene trinitramine), PETN (pentaerythritol tetryanitrate) and TNT (2,4,6-trinitrotoluene) were placed in a steel container (18 × 18 × 18 cm\(^3\)) and detonated (during separate explosions) at Advanced Materials Engineering Pte Ltd (AME) (Singapore) facility by the trained staff. Especially designed sample catchers (Banas et al. 2009) were used in order to maximize the number of residues obtained after each explosion. All post-blast residues

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were collected in separate plastic bags and transported to the laboratory at Singapore Synchrotron Light Source (SSLS).

Fourier transform infrared (FTIR) spectroscopy analysis was performed at SSLS (Bahou et al. 2007) with spectrometer Bruker type IFS66V/s (Bruker Optics Inc). During all measurements the mercury cadmium telluride (MCT) detector cooled to liquid nitrogen temperature was used. The sample compartment was evacuated down to 300 Pa to avoid the influence of air in the final spectrum. All spectra were collected within the frequency range of 4000 to 600 cm$^{-1}$ in transmission mode at the resolution of 4 cm$^{-1}$. Multiple spectra were acquired on each sample in order to determine the reproducibility. Six hundred scans were averaged to obtain good signal-to-noise ratio. Samples of residue materials were prepared by sweeping the surface with a cotton stick soaked with acetone. Traces of the explosives were separated from the solvent by evaporation, and after that mixed with potassium bromide (KBr) ground to fine powder and pelletized under a hydraulic press with a clamping force of 80 kN. More than 200 samples containing residue materials collected from various surfaces of objects that were within a close distance from the centre of explosion were prepared. Appropriate data treatment was used before the multivariate analysis (Banas et al. 2010).

2. Results

Among many multivariate statistical techniques hierarchical cluster analysis and principal component analysis (PCA) seem to be most adequate for spectral data mining. After trials and comparison of the obtained results we decided to use Euclidean distance as the proximity measure. Single, complete, average linkage and Wards’ algorithm were tested as the aggregation methods. Example of cluster analysis on reference spectra of four pure explosives materials by using Wards’ algorithm is presented in figure 1; four well separated clusters associated with

![Cluster Dendrogram](attachment:image.png)

**Figure 1.** Result of hierarchical cluster analysis on reference spectra (Wards’ algorithm).
four various explosive materials are clearly visible. PCA was applied to a set of data containing the spectra of four pure explosive materials and the spectra of residues collected after the blasts. R platform for statistical computing and graphics was used in the calculations (package stats) (R Development Core Team 2010). More than 99.6% of the total variance was explained by the first three PCs, while the other PCs were related to the non-significant part of the total variance. Figure 2 shows the resulting score scatter plot for the first and second principal component obtained for the analysis of the data collected after all three trials. Three distinct clusters are apparent in the graph. As one can see very good separation and unambiguous identification of the high energetic material used during each trial is possible by using this method.

3. Conclusions

The major problem in contemporary spectroscopy is to find the ways of dealing with large number of correlated variables. The aim of analysing data is often to find...
the underlying structure of a system and to describe it in the simplest possible way. Spectroscopic measurements have the capacity to provide a lot of data in a short time, giving a chemical and physical description of the observed samples. However, due to the complexity and high similarity of obtained spectra special multivariate statistical methods have to be used in data evaluation.

In comparison with conventional practice FTIR spectroscopy combined with multivariate analysis has several advantages: it has the potential for fully automatic measurement and analysis, it is very sensitive and very small samples are adequate, and it is potentially much quicker and cheaper for large-scale screening procedures.

REFERENCES


