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The Investigation into Interactions Between Explosive Residue and Common Household Cleaning Supplies Using Infrared Spectroscopy

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This project investigated the interactions between explosive residue and common household cleaning supplies using Infrared Spectroscopy (IR). IR has been used before to analyze explosives and Castro-Suarez et. al. states that vibrational techniques, such as IR, are useful in the identification of explosives, considering each chemical substance has their own unique, or "fingerprint", spectrum. The goal of this project was to investigate how various common cleaning products (Clorox, Lysol, Simple Green, Windex, Pledge, Murphy Oil Soap, Resolve) would affect the IR spectrum of different explosives (RDX, TNT, PETN, and TATP). The explosives were used in the pre-packaged solution. The RDX and TNT were 1000 ug/mL in MeOH:AcCN (50:50), PETN was 1000 ug/mL in Methanol, and the TATP was 0.1 mg/mL in AcCN. Spectra of the cleaning agents and the explosives alone were obtained and compared to spectra of mixtures of explosives and cleaning agents. The preparation of the cleaning agents included cutting out plastic films, applying 3 drops of cleaning agent, and allowing them to dry overnight in the fume hood. The explosives (5 uL) were pipetted directly onto the IR stage and analyzed immediately once the solvent evaporated. To prepare the mixtures, 5 uL of the explosives were pipetted onto plastic films and allowed 15 minutes to dry, then 3 drops of the cleaning agent were applied to the dried explosive, and dried overnight in the fume hood. Three slides of each sample were prepared and each were run in triplicate on the IR, so there were 9 runs total for each mixture of cleaning agent and explosive. The resulting spectra from the mixture of the cleaning supplies with the explosives were compared to the spectra of the explosives and cleaning supplies alone to determine if there could have been a reaction between the explosives and the added cleaning agent. Statistical analysis was then conducted to determine if the changes were significant.

The results were as hypothesized; the cleaning agents did have an effect on the IR spectrum of the explosives. The explosive that displayed the most change was RDX in the presence of Simple Green, however notable changes were also observed within the PETN and Clorox mixture, and similar changes were observed for most other explosives and cleaning agent combinations. The observed changes were differences in the percent transmittances of signature IR peaks in the explosives spectrum, which could indicate either the breaking or formation of bonds due to a reaction between the two samples, a suppression of the explosive by the cleaning agent, or the removal of the explosive from the surface. There are no plans for publication, as further research is required to identify what could have caused these observed changes. Further research includes running mass spectrometry to identify the cause of these changes, including identifying possible new compounds or adducts formed due to a chemical reaction, running wet slides instead of allowing them to dry, and running Raman Spectroscopy instead of IR to compare these two nondestructive vibrational analytical techniques.

References:

Castro-Suarez, J. R.; Pacheco-Londono, L. C.; Aparicio-Bolano, J.; Hernandez-Rivera, S. P. Active Mode Remote Infrared Spectroscopy Detection of TNT and PETN on Aluminum Substrates. Journal of Spectroscopy 2017, 2017, 1–11.