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

Alyson Shaw & Alyssa Marsico, Ph.D.
Department of Forensic Science, University of New Haven, West Haven CT.

Overview

- The interaction of explosives with cleaning agents was investigated using infrared (IR) spectroscopy.
- Changes in percent transmittance (%T) were observed, possibly indicating the formation of new bonds or breaking of bonds.
  - RDX + Simple Green displayed the greatest change in %T.
  - PETN + Clorox also displayed significant changes.
  - Similar changes were observed for other explosives and cleaning agents.

Introduction

- Positive identification of explosives pre-blast is important because it will inform the investigators that someone was in contact with explosives.
- Contamination of explosives at a crime scene is likely, which could prevent positive ID of the explosives at the scene.
  - Such contamination can be from an attempt to clean up explosive residue with common household cleaning agents.
- A mixture of common household cleaning agents with explosive residue could cause adducts to form, indicating that a chemical reaction has occurred and a new compound has been made.
  - If a new compound is made, then it might mask the presence of explosive residue and may cause a preliminary explosive test to fail. This could be misleading to an investigation.
- Spectroscopy has been used previously to identify explosives. One type that is used is IR spectroscopy. IR spectroscopy is rapid, non-invasive, and provides a multiplex advantage[1]. It has been proven to be useful in the identification of explosives since each chemical substance has its own unique spectrum[2].

Methods

- Cleaning agents (7): Simple Green all-purpose cleaner, Clorox splash-less bleach, Windex multi-surface, Pledge multi-surface cleaner with glade, Lysol, Murphy oil soap wood cleaner, Resolve stain remover.
- Explosives (4): RDX 1000 µg/mL in MeOH:ACN (50:50), PETN 1000 µg/mL in Methanol, TNT 1000 µg/mL in MeOH:ACN (50:50), TATP 0.1 mg/mL in ACN
- Baseline spectrums of the cleaning agents and the explosives alone were collected; three samples were run three times each for each cleaning agent and explosive.
  - The cleaning agents were prepared by placing three drops of the cleaning agent from a transfer pipette into the center of a plastic slide. The slides were dried in a fume hood overnight and spectra were collected after dry.
  - The explosives were prepared by pipetting 5 µL of the solution directly on the IR stage and collecting the spectra immediately.
- The mixtures were prepared by depositing 5 µL of the explosive solution onto the plastic slide and allowing it to dry for 15 minutes. Three drops of the cleaning agents were applied to the explosives. The slides were dried overnight in the fume hood and the spectra were collected after dry.
- The baseline spectra were compared to the mixture spectra to observe any changes in the percent transmittance of the peaks present.
- Statistical analysis was then conducted to determine if any of the changes were significant.

Results

- RDX + Simple Green displayed significant differences compared to the baselines.
  - A carbonyl peak arises after the mixture, which may have been constricted before.
  - Other new peaks are seen, as well as an increase in %T in the fingerprint region. This indicates that new bonds have been formed.
- PETN + Clorox also displayed increases in %T indicating that new bonds have been formed.
  - New peaks corresponding to a nitro compound and S=O compound are observed.
- TNT + Pledge had an overall decrease in %T, indicating that bonds have been broken.
  - The nitro compound peak in TNT alone is not present in the mixture spectra.
- TNT + Murphy Oil Soap had an overall decrease in %T, while TNT + Resolve had an overall increase in %T.

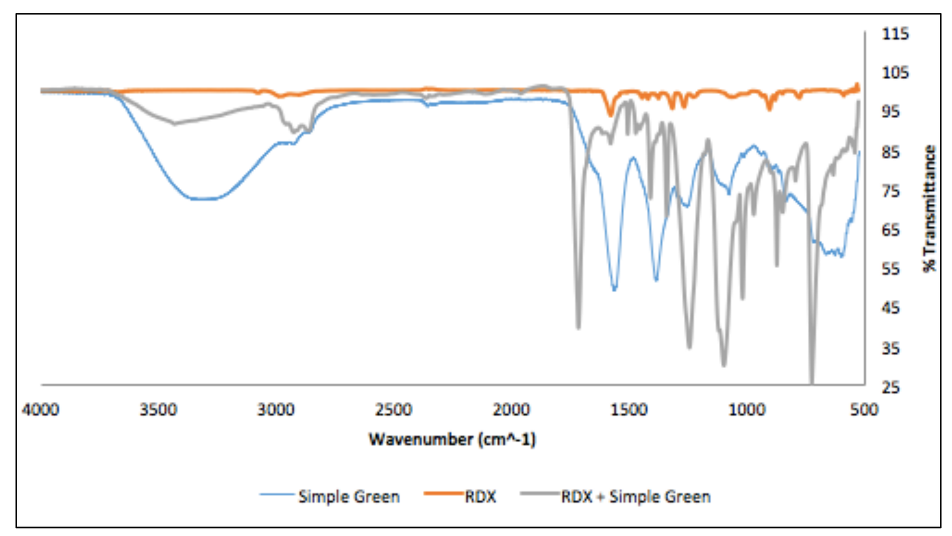

Figure 1: Spectra of RDX + Simple Green

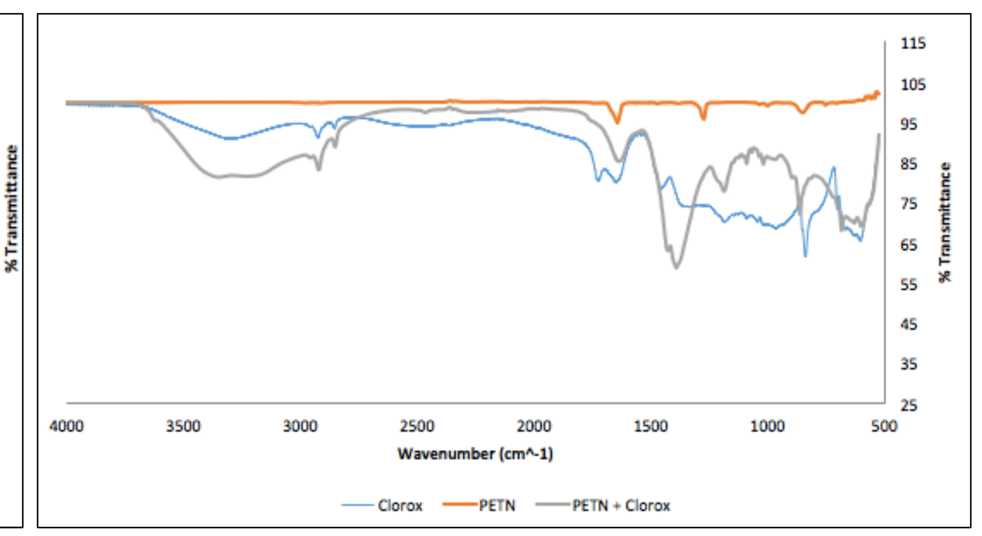

Figure 2: Spectra of PETN + Clorox

- When further investigating the carbonyl peak of the Simple Green mixtures, TNT and TATP mixtures also displayed a decrease in %T.
- The S=O peak in the Clorox mixtures displayed an increase in %T for TNT and RDX.
  - The PETN mixture had a decrease in %T.
  - The TATP mixture had relatively no change in %T.
- The CN stretching in the Pledge mixtures indicated a decrease in %T for RDX, TATP, and PETN.
  - There was an increase in %T for TNT only.
- The methyl stretching in the Resolve mixtures showed a decrease in %T in mixtures of all of the explosives.

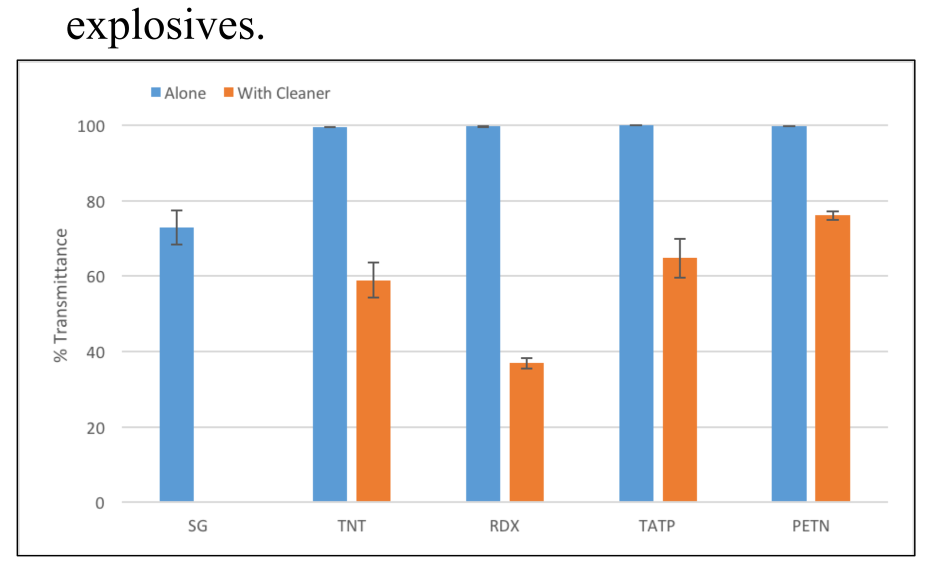

Figure 3: Average Percent Transmittance for carbonyl stretching (1710 cm^{-1}) in Simple Green Mixtures

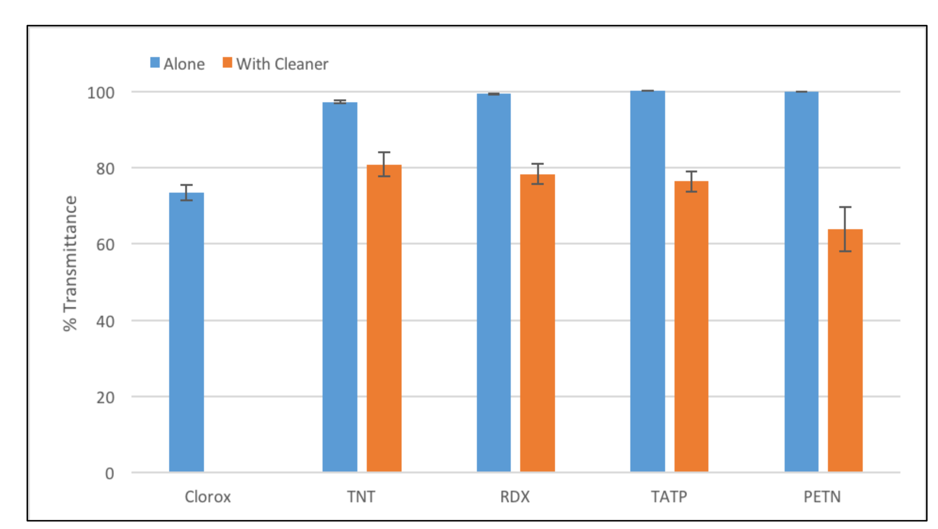

Figure 4: Average Percent Transmittance for S=O stretching (1360 cm^{-1}) in Clorox Mixtures

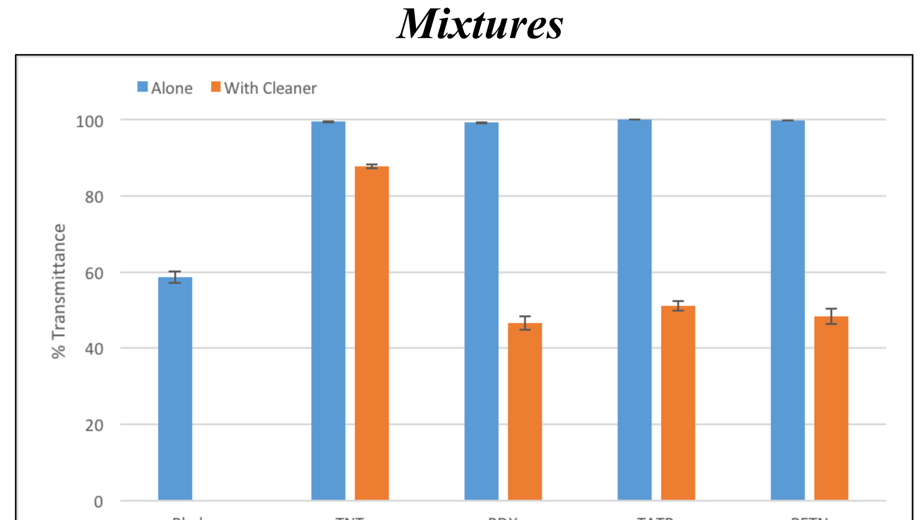

Figure 5: Average Percent Transmittance for CN stretching (1241 cm^{-1}) in Pledge Mixtures

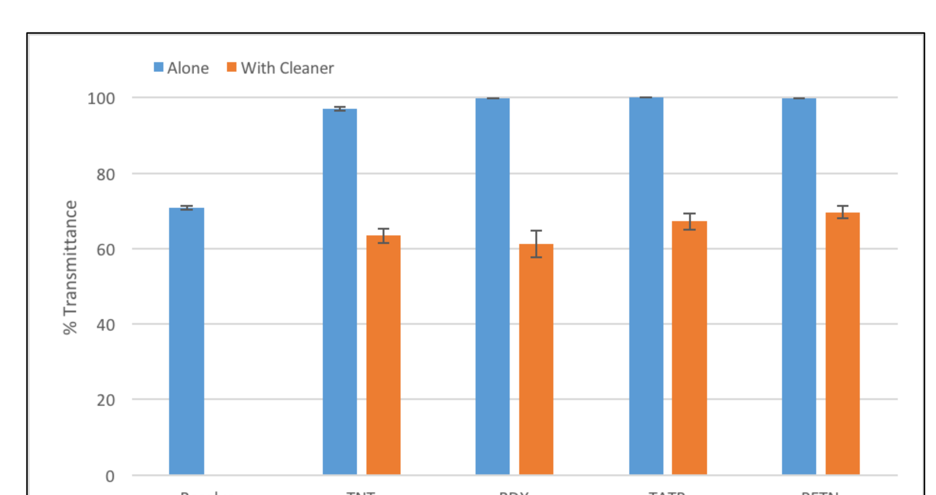

Figure 6: Average Percent Transmittance for methyl stretching (720 cm^{-1}) in Resolve Mixtures

Conclusions

- We observed the interaction between explosive residue and cleaning agents using IR spectroscopy.
  - The increases in %T could be due to decreases in vibrational signals as a result of new bonds forming.
  - The decreases in %T could be due to increases in vibrational signals as a result of bonds breaking or loosening up.
- The peaks corresponding to S=O compounds account for most of the new peaks formed during the mixtures.
  - This was found in most of the cleaning agents since soaps are common ingredients in the cleaning agents.
- The peaks corresponding to the nitro compounds displayed variations in %T among the mixtures.
  - After some mixtures the peak became absent, while during other mixtures the peak was newly formed.
- Changes in the transmittance of the methyl peaks were seen in most of the mixtures of the cleaning agents with the explosives.
- The Simple Green mixtures with RDX and TNT displayed the most significant changes in %T.
  - The explosives showing the most change were RDX and TNT.
  - The cleaning agent showing the most change was Simple Green.
- PETN and TATP did not show significant changes in any of the combinations with most other cleaning agents.

Future Directions

- Using mass spectrometry to identify any new compounds or adducts formed when mixing explosives and cleaning agents.
- Investigate other methods of mixing the explosives and cleaning products.
  - Depositing the explosives on a surface and then using the cleaning product to clean the surface.
  - Analyze wet samples rather than allowing the samples to dry before analysis.
- Use Raman spectroscopy for the same experiments to compare nondestructive methods.

References

1. Gautam, R.; Samuel, A.; Sil, S.; Chaturvedi, D.; Dutta, A.; Ariese, F.; Umapathy, S. *Raman and mid-infrared spectroscopic imaging: applications and advancements.* Current Science 2015, 108, 341–356.
2. 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.

Acknowledgments

I'd like to thank Carol Withers, Lynne Resnick, and the rest of the SURF committee for giving me the opportunity to conduct my research. I'd like to thank my mentor, Dr. Marsico, for guiding me through this project. Lastly, I'd like to thank Sandra Hartmann-Neumann and the rest of the Forensic Science Department for allowing me to use the lab space needed to conduct my research.