

**Characteristic TNT Differential Reflection Spectra on Common Substrates**

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### Abstract

This work describes an explosives detection technique utilizing differential reflectograms to identify the characteristic differential reflectivity spectra of TNT. It accomplishes this by measuring the characteristic differential reflectivity (essentially the absorption) of a specimen while being exposed to high intensity UV light. The differential reflectometer is able to achieve high sensitivity because it measures two adjacent parts of the specimen simultaneously. As a result, a normalized difference in reflectivity is recorded and trace quantities of materials become apparent. It is shown that traces of 2,4,6-trinitrotoluene (TNT) display a characteristic shoulder in differential reflectograms in the optical spectral range of 380-420 nm. This characteristic shoulder is not obscured if TNT is deposited on fabrics, luggage, office supplies, human skin, metallic foil, or various papers and plastics. These substrates were tested because they are typical materials seen by airport terminal security systems. Wood, particle board, and plywood showed characteristic features in the same spectral range as TNT. They are, however, considerably weaker than that for TNT. It is not anticipated that these substrates will conceal the TNT signature to such a degree as to camouflage it from detection or cause a false positive. In short, differential reflectometry is shown to be a contactless, portable, and inexpensive optical detection system which detects TNT (and other explosives) on a large number of common substrates and can therefore be used where a high degree of security is needed, such as in airport security scanning devices.

### Introduction

The purpose of this work is to describe an explosives detection technique that promotes a high degree of security, specifically in airport terminals where safety is a priority. As mentioned above, differential reflectometry can be utilized to detect minute amounts of explosives across the surface of a broad range of specimens. It accomplishes this by measuring the characteristic differential reflectivity (essentially the absorption) of a specimen while being exposed to high intensity UV light. The differential reflectometer is able to achieve high sensitivity because it measures two adjacent parts of the specimen simultaneously. As a result, a normalized difference in reflectivity is recorded and trace quantities of materials become apparent (Hummel et al. 2006).

Current detection mechanisms in use can be categorized into several principles of operation: ionization and separation analysis of the explosive vapor; pyrolysis and gas-phase reactions; bulk detection by means of a reaction of an incident radiation with an element or elements of the explosive compound; and, detection of a product of a biochemical reaction with the explosive (Yinon 2002). Ion mobility and mass spectrometer based chemical sniffers (Yinon 2003) as well as gas chromatographs (GC) with electron capture detectors (ECD) and thermal energy analyzers (TEA) (Hodyss et al. 2005) have a high sensitivity but require a vapor sample and are slow to analyze the sample (Yinon 2002). Radiation

based instruments such as x-ray machines, computer tomography (CT) scanners, and pulse induction metal detectors have the advantage of being contact-less, but are bulky and expensive. In addition, x-rays and CT scanners rely on density determination to identify possible explosives. This creates a high number of false positives. Low-tech methods such as K-9 unit police dogs and manual searches are time consuming as well as labor intensive (St. John 1991).

This is why there is a high demand for faster, cheaper, and more efficient explosive detection devices. Techniques in development are broad but can be sub-divided into three classes: vapor and particle detectors; radiation detectors; and, biochemical /electrochemical detectors (Yinon 2002). Radiation detectors comprise the broadest and conceivably most effective group. Nuclear quadrupole resonance (NQR) (Yinon 2002), pulsed laser surface fragmentation and mid-infrared laser spectroscopy (Bauer et al. 2006), frequency modulation spectrometry (Riris et al. 1996), terahertz spectroscopy (Shen et al. 2005), and Raman spectroscopy (Carter et al. 2005) are all in development to be adapted for explosives detection. Neutron analysis (Eberhardt et al. 2005) is also being improved upon, as the current machines are large, non-portable, and expensive. Fiber-optic laser sensors are being considered for mine detection (Bohling et al. 2006), and have the potential to be adapted for airport security

applications as well. The primary advantage of radiation-based detection mechanisms is that they are contact-less, without the need to hire manpower for swabbing, searching, or handling a bag. This non-intrusive method allows for quicker security checkpoints and reduced costs. It also reduces the possibility for human error.

Although a number of biochemical (Yinon 2002), electrochemical (Yinon 2002), and polymer (Toal and Troglor 2006) detectors exist, these are suited for explosive detection in soil and water samples and have not been developed with security in mind.

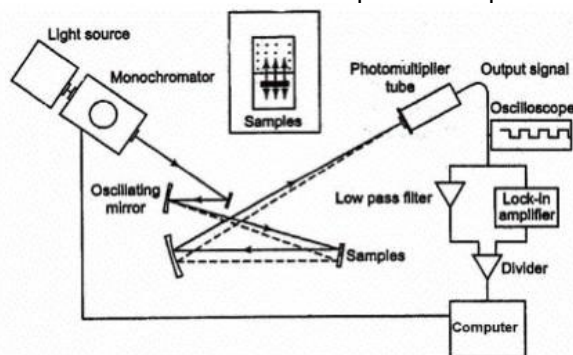
Among the optical detection mechanisms discussed, differential reflectometry (DR) is a potentially superior technique. It can be incorporated into already existing airport systems, is contact-less, fast, and cost effective. A differential reflectometer will detect, at a distance, traces of chemical explosives or narcotics on a passenger or piece of luggage (Hummel et al. 2006). It does this quickly and accurately with minimal false positives. In addition to airport terminals, differential reflectometry has further applications in sports stadiums, markets, train stations, military installations, and embassies, where threats from car bombs, chemical weapons, and suicide bombers are prevalent. Ideally, differential reflectometry can identify a potential threat before it comes within a dangerous distance of a facility.

In the reported experiments, differential reflectometry is used to ascertain a baseline differential reflectivity spectrum of various substrates, materials where explosives residue may be present, to determine if they interfere with the characteristic differential reflectivity spectrum of 2,4,6-trinitrotoluene (TNT) a common high explosive. This data can be applied to future DR based explosives detection machines utilized for military and airport security. In a situation such as airport security, a detection machine will be exposed to a myriad of substrates. Because of this, laboratory tests must be performed to ensure no common substrates constitute a security weakness by masking the TNT signature. In addition, substrates must be tested to determine which, if any, resist adhesion of TNT and therefore will not maintain a measureable TNT residue after being handled or exposed to the explosive.

### Materials and Methods

The instrument light source is a high intensity, high-pressure xenon bulb. Light from this bulb is shone into a monochromator where it is emitted as non-polarized, monochromatic light. The

monochromator steps the wavelength of the light from 200 nm to 500 nm at a speed of 200 nm/minute during any given test. The light then reaches an oscillating mirror where it is alternately deflected onto the two areas of the sample being measured. A typical total measured area on the sample is 2x4 mm<sup>2</sup>. After being reflected off the sample, the light reaches a stationary mirror where it is directed onto the face of a photo-multiplier



**Figure 1: Components that comprise the differential reflectometer (Hummel 1988).**

tube (PMT). The PMT converts the collected light into an output voltage that is sent to a lock-in amplifier (LIA) and a low pass filter. The signal is then passed through a divider to a computer where it is digitized and plotted vs. wavelengths. This yields different reflectivities. Figure 1 illustrates this instrument (Hummel 1988).

A normalized difference is calculated from  $R_1$  and  $R_2$ , which are the reflectivities of the two measured areas of the sample. The difference in reflectivity ( $\Delta R = R_2 - R_1$ ) is provided by the LIA and the average reflectivity ( $R_{avg} = [R_1 + R_2] / 2$ ) is provided by the low pass filter. A ratio,  $\Delta R / R_{avg}$ , is achieved

|                                       |   |
|---------------------------------------|---|
| Felt                                  | Particle Board                            |
| Velvet                                | Plywood 1                                 |
| Denim                                 | Plywood 2                                 |
| Airport wipe                          | Brown Paper Towel                         |
| Cotton                                | Brown Paper Towel with yellow highlighter |
| Cotton/Poly Blend                     | Ziploc Bag 2                              |
| Nylon (Black)                         | Business Card                             |
| Eyeglass wipe                         | Business Card 2                           |
| Acetate                               | Dielectric Ceramic                        |
| Nylon (Blue)                          | Highlighted yellow sticky note            |
| Jansport Backpack sample (Matte side) | Black garbage bag                         |
| Jansport Backpack sample (Shiny side) | Blue Highlighter on white paper           |
| Human finger                          | Patterned fabric cotton sample 1          |
| Dried Elmers glue on paper            | Patterned fabric cotton sample 2          |
| Kimwipe sheet                         | Patterned fabric polyester sample         |
| Ziploc bag 1                          | Synthetic leather sample                  |
| Light office chair wood               | Aluminum foil sample                      |
| Pine Wood                             |   |

**Table 1: Substrates tested throughout the course of experimentation**

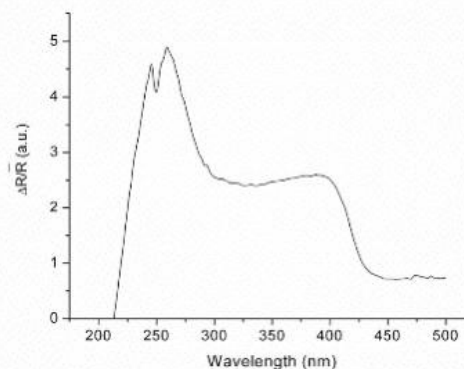
when the signal passes through the divider. By measuring  $R_1$  and  $R_2$  at the same time and forming a ratio, possible errors due to line voltage fluctuations, intensity fluctuations from the light source, spectral sensitivity variations in the detector, and the spectral reflectivity of the mirrors and substrate are eliminated (Hummel et al. 2006). Although the DR measures the reflected light, the data it reports is proportional to the sample absorption. The energies that electrons absorb from incident photons as they are raised into higher, allowed energy states are measured. Because each material has characteristic electron transitions, this absorption pattern serves as a fingerprint for identifying the material (Hummel 1983). The substrates tested can be found in Table 1.

A procedure is strictly followed during testing to ensure accurate and consistent results. After the instrument assembly is powered on and the xenon lamp lit, at least two control tests are run to ensure the equipment is warmed up and functioning properly. The computer steps the grating from 200 nm to 500 nm and records the difference in reflected light. Generally, three tests are run before the sample is adjusted so that the light shines onto a different area of the sample. Another three tests are then run and the sample is changed. Each set of three tests is averaged and plotted with the averaged results from the second spot on a particular sample. All samples are tested first without TNT, and then with TNT to provide a baseline measurement and control for comparison. All tests are run at approximately sea level, 1 atm, and room temperature.

### Experimental Results

Experiments began with TNT samples tested on carbon pads. Because carbon pads have essentially no features in the range of interest, this allowed the determination of TNT's characteristic differential reflection spectrum.

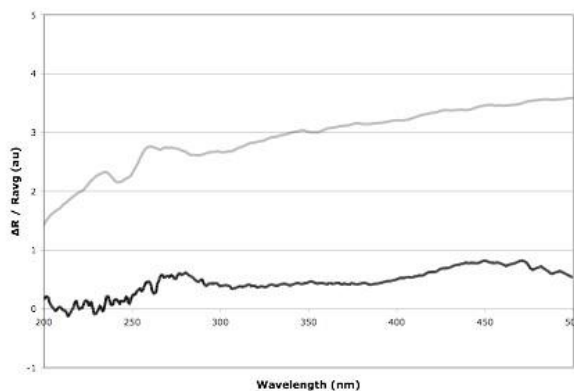
Figure 2 shows this characteristic differential reflection spectrum (Hummel et al. 2006). This is the spectrum that is looked for among all the substrates tested. Specifically, the shoulder seen at 380-420 nm is most identifiable. If this shoulder is clearly evident, a result is considered positive. This shoulder is identified by a proprietary computer program. None of the tested substrates showed a definitive interference with the characteristic spectrum of TNT. However, some substrates partially obscured the TNT signature. It is not anticipated that these substrates will conceal the TNT signature to such a degree as to camouflage it



**Figure 2: Characteristic TNT differential reflection spectrum (Hummel et al. 2006).**

from detection. In addition, no substrates were found to resist adhesion of TNT.

Figure 3 shows a Jansport backpack sample tested without the presence of TNT to obtain a baseline measurement for that material. Note that no features characteristic to the backpack material exist that might mask the TNT

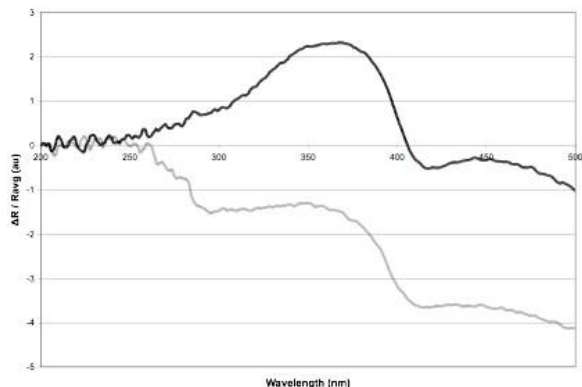


**Figure 3: Jansport backpack sample (Matte side) tested without TNT. The darker line is spot 1 and the lighter line is spot 2.**

signature seen in Figure 2. Figure 4 shows the same sample tested with the presence of TNT.

The shoulder around 400 nm that identifies the TNT is clearly visible in Figure 4. The Jansport sample without TNT failed to exhibit any significant absorption features in the 380-420 nm range. In Figures 5-33 the results of various substrates with (dark lines) and without TNT (light lines) are depicted (See Appendix for Figures 5-33).

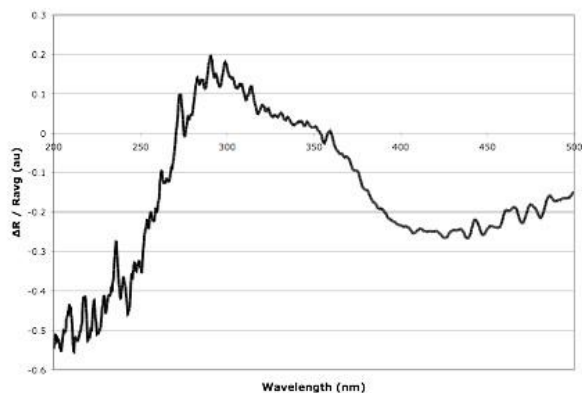
Figure 34 shows a piece of wood chiseled from an office chair tested without TNT. There is a small shoulder evident from 360-400 nm. This does not mask the TNT signature, however, it may partially obscure it. Figure 35 shows the same



**Figure 4: Jansport backpack sample (Matte side) tested with TNT. The darker line is spot 1 and the lighter line is spot 2.**

substrate tested with the presence of TNT. The TNT shoulder is again evident but much larger than the characteristic shoulder of the plain wood, however, it is shifted to a lower wavelength. This is cause for concern because it could potentially interfere with the detection process. Further testing and possible adjustments will have to be made to a detection software to ensure this type of shifting does not allow TNT to pass undetected.

Figure 36 (Appendix) shows a comparison of four other wood samples tested both with and



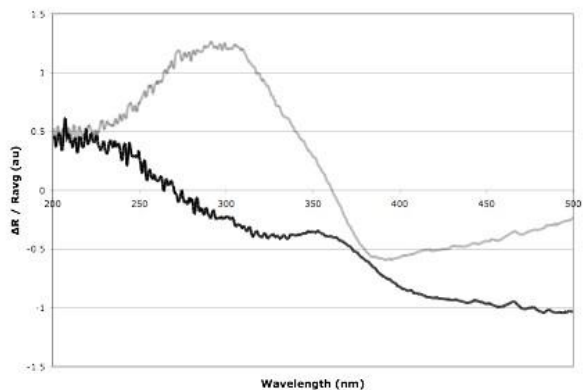
**Figure 34: Light wood from office chair tested without TNT.**

without TNT. The dark lines in the graphs are the tests performed with TNT, while the lighter lines are without TNT.

## Discussion

Differential reflectometry has the potential to surpass current optical detection techniques in regard to speed, accuracy, and cost. It will detect, without contact, traces of chemical explosives (or narcotics) on passengers or pieces of luggage (Hummel et al. 2006). It does this with minimal false positives and operator training. In addition to

airport terminal security, it has further applications in military and embassy security where car bombs, chemical weapons, and suicide bombers are all potential threats.



**Figure 35: Light wood from office chair tested with TNT. The darker line is spot 1 and the lighter line is spot 2.**

During testing, a baseline reflectivity for TNT was clearly established, and a multitude of substrates were determined to not interfere with TNT detection. These substrates showed a high degree of clarity in the TNT signature. The only substrates that showed a characteristic shoulder similar to TNT were wood samples. Particle board in particular showed a propensity to diminish the TNT signature. Particle board is manufactured by grinding many types of wood into small, fine chips and then gluing them together with an industrial epoxy process. Because of this, the differential reflectometer receives many different reflectivities from the two areas of the substrate measured. This tends to hide any trace materials present on the substrate. Also, the ground wood chips provide many refraction angles which scatter the incident UV beam and diminish the amount of light received by the PMT for measurement. The first plywood sample showed a shoulder very similar to TNT but blue shifted by approximately 30 nm and with a more gradual slope. When compared to a test run with TNT present, the difference was evident, but tested without TNT the plywood may cause a false positive. The Pine wood showed the same characteristic shoulder however the slope was considerably less steep. The wood and particle board samples did not completely mask the TNT signature. It is believed that the detection software can be adjusted to accommodate these substrates and remedy this interference, preventing false positives. Because the measured reflectivity is differential in nature, a substrate with a high absorption will not mask the TNT signature. Rather, it will only lessen the intensity of the TNT

signature by allowing less light to reach the PMT in a particular spectral region. To mask TNT, a substrate must exhibit similar absorption features to TNT in the same spectral region.

Possible sources of error in these tests include human error, such as placing the incident UV beam on an area of the sample where no TNT is present. Sources also include instrumental error such as noise in the equipment or a malfunctioning data acquisition card. Another possible error source is ambient light reaching the sample during testing. Human error can be remedied with careful inspection of the samples and the location of the UV beam when securing a sample prior to a test. Instrumental error can be reduced by testing at least two control samples before starting measurements. The anticipated final concept for the DR calls for many consecutive tests on a given substrate to be performed in varying areas on that sample, which should further eliminate any appreciable instrumental error.

As determined by the experimental data, it has been shown that the differential reflectometer can test materials in a variety of cases. After being manufactured into a more compact, portable design, it can be integrated into airport security devices to provide a contactless, fast, and effective scanning device. This will increase both ease and safety of travel. It can also be implemented into embassy and military security systems. In a hostile environment, where the threat of terrorist bombing is ever present, a contactless and reliable scanning device can prove invaluable.

## References

Bauer C, Geiser P, Burgmeier J, Holl G, Schadel W (2006) Pulsed laser surface fragmentation and mid-infrared laser spectroscopy for remote detection of explosives. *Appl. Phys. B* 85: 251-256.

Bohling C, Scheel D, Hohmann K, Schade W, Reuter M, Holl G (2006) Fiber-optic laser sensor for mine detection and verification. *Applied Optics* 45: 16: 3817-3825.

Carter JC, Angel SM, Lawrence-Snyder M, Scaffidi J, Whipple RE, Reynolds JG (2005) Standoff Detection of High Explosive Materials at 50 Meters in Ambient Light Conditions Using a Small Raman Instrument. *Applied Spectroscopy* 59: 769-775

Eberhardt JE, Rainey S, Stevens RJ, Sowerby BD, Tickner JR (2005) Fast neutron radiography

scanner for the detection of contraband in air cargo containers. *Applied Radiation and Isotopes* 63: 179-188.

Hodyss R, Beauchamp JL (2005) Multidimensional Detection of Nitroorganic Explosives by Gas Chromatography-Pyrolysis-Ultraviolet Detection. *Analytical Chemistry* 77: 3607-3610.

Hummel Rolf E (1988) Differential Reflectometry and its Application in Materials Science. *Surface and Interface Analysis* 12: 1: 11-14.

Hummel Rolf E (1983) Differential Reflectometry and Its Application to the Study of Alloys, Ordering, Corrosion and Surface Properties. *Physica Status Solidi (a)* 76: 1: 11-44.

Hummel Rolf E, Fuller A, Schollhorn C, Holloway P (2006) Detection of Explosive Materials by Differential Reflection Spectroscopy. *Applied Physics Letters* 88: 231903.

Riris H, Carlisle CB, McMillen DF, Cooper DE (1996) Explosives detection with a frequency modulation spectrometer. *Applied Optics* 35: 24.

Shen YC, Lo T, Taday PF, Cole BE, Tribe WR, Kemp MC (2005) Detection and identification of explosives using terahertz pulsed spectroscopic imaging. *Applied Physics Letters* 86: 24: 241116.

St. John P (1991) Air Piracy, Airport Security, and International Terrorism: Winning the War Against Hijackers. Quorum Books.

Toal SJ, Trogler WC (2006) Polymer sensors for nitroaromatic explosives detection. *Journal of Materials Chemistry* 16: 2871-2883.

Yinon J (2002) Field detection and monitoring of explosives. *Trends in Analytical Chemistry* 21: 4: 292-301.

Yinon J (2003) Detection of Explosives by Electronic Noses. *Analytical Chemistry* 75: 5: 98A-105A.

## Appendix

Figures 5-33: Results of various substrates tested with and without TNT. The darker lines are with TNT and the lighter lines are without TNT. Figure numbers are indicated in the lower left corner of each graph. Note: Some graphs show only substrates without TNT.

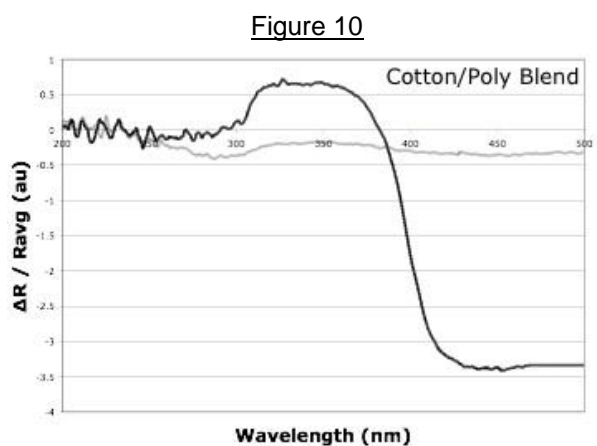
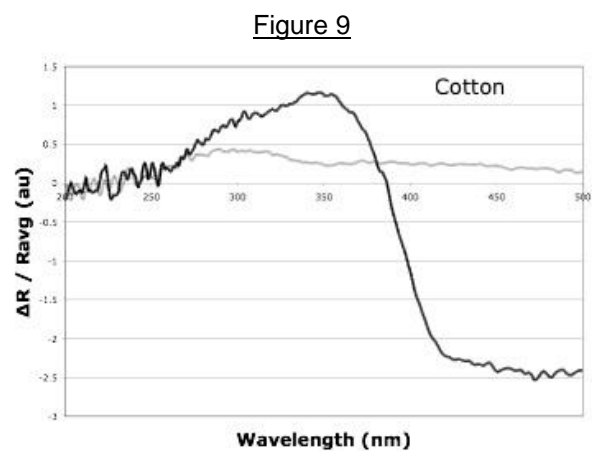
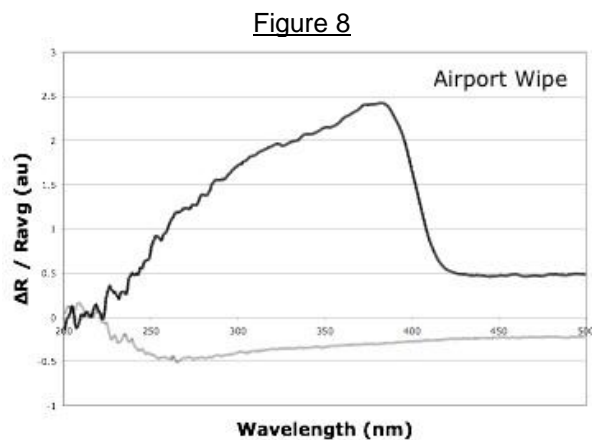
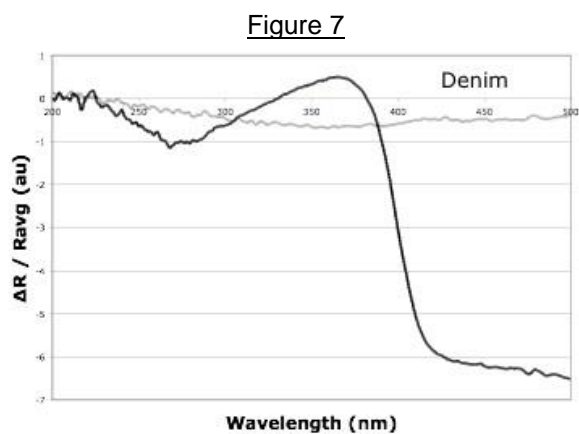
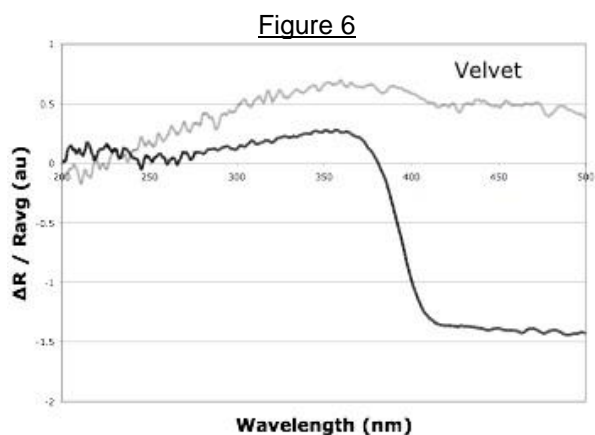
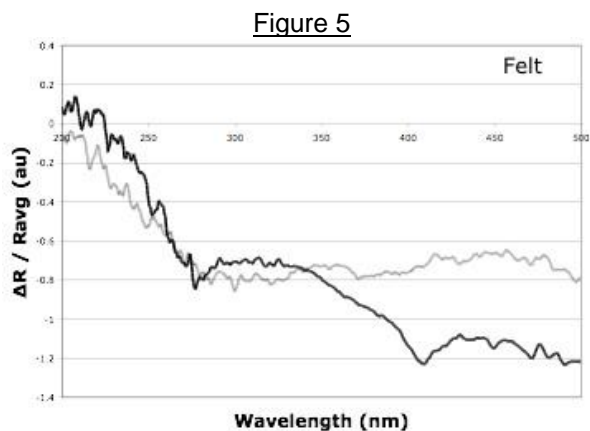


Figure 11

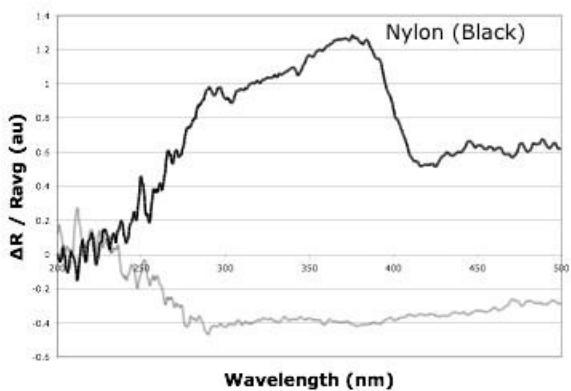


Figure 14

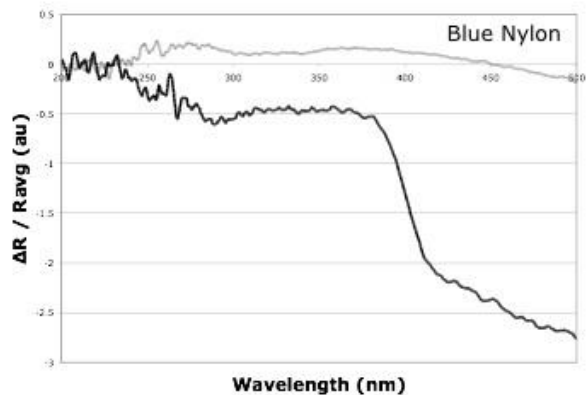


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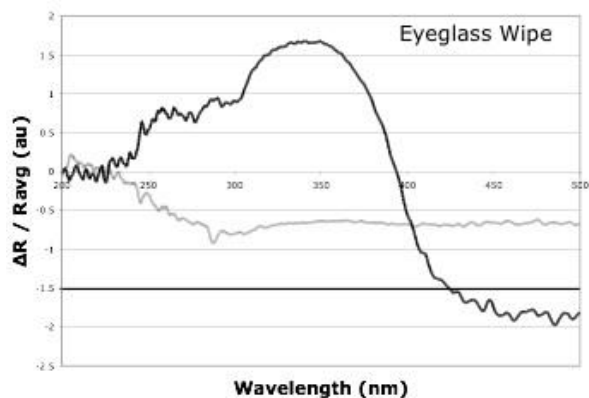


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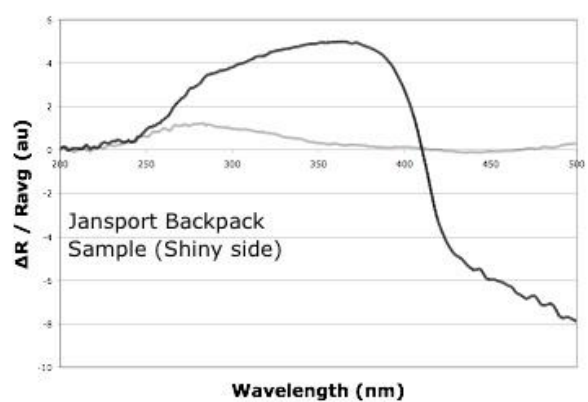


Figure 13

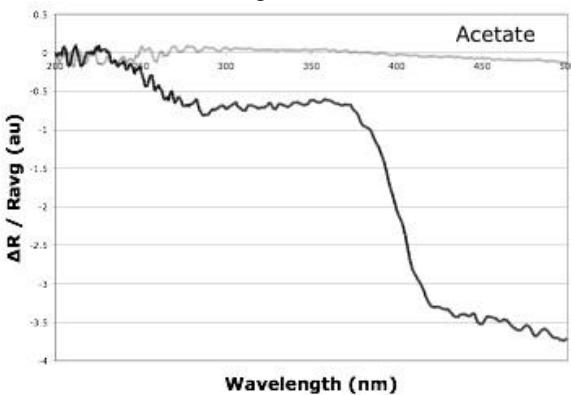


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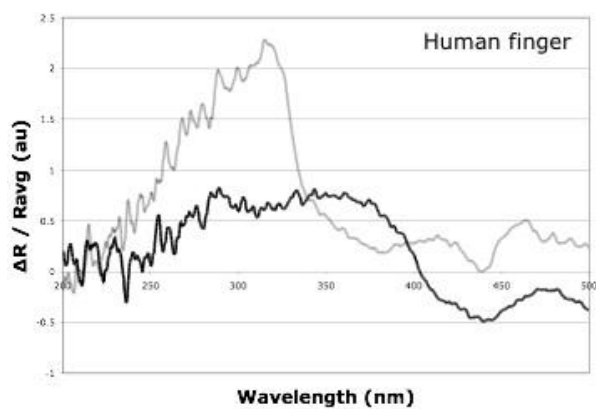




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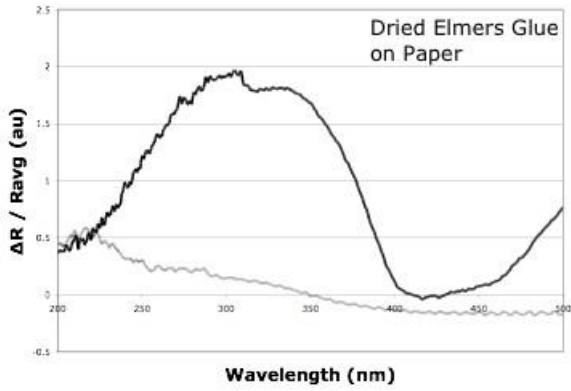


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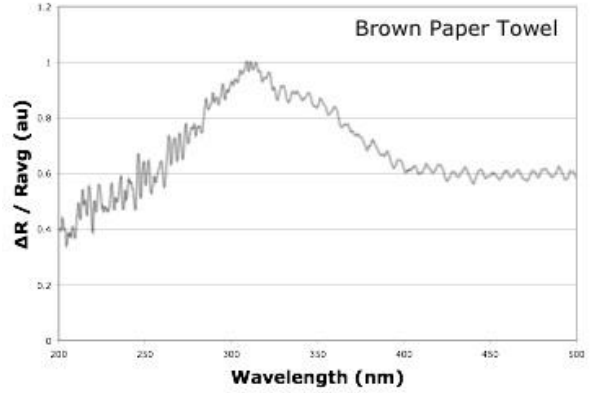


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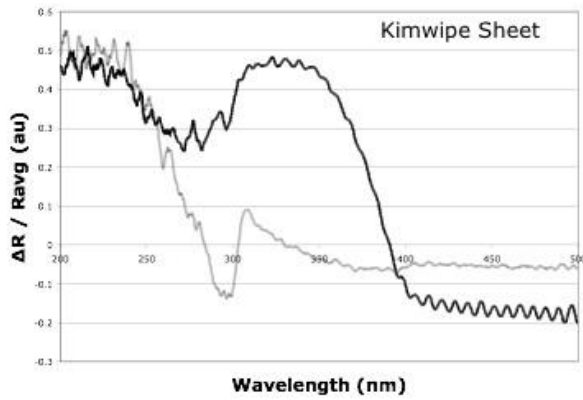


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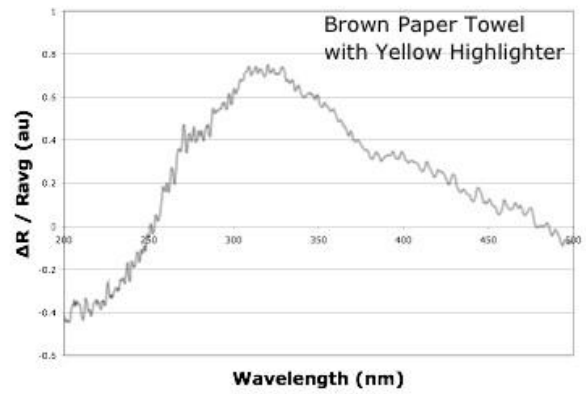


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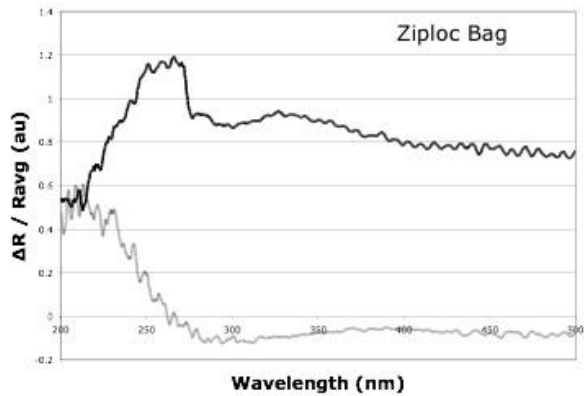


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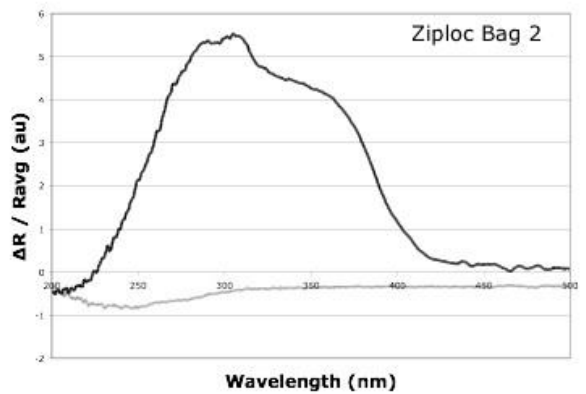


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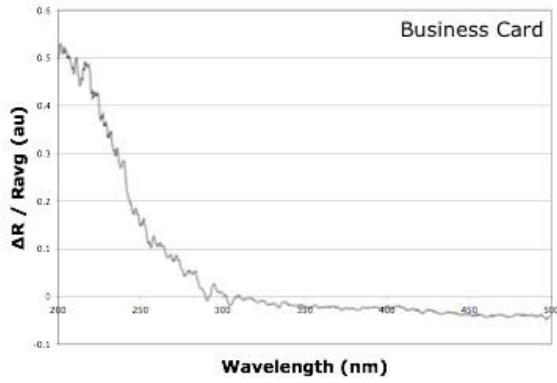


Figure 26

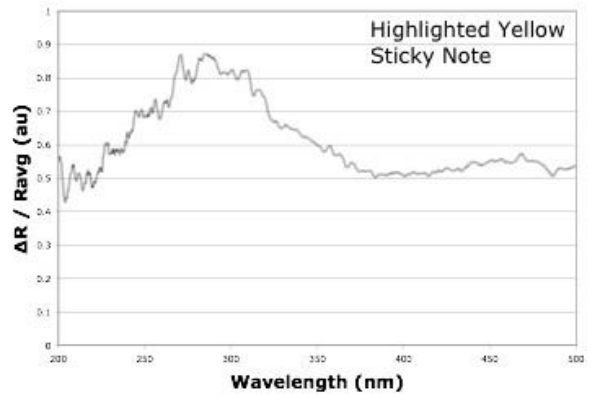


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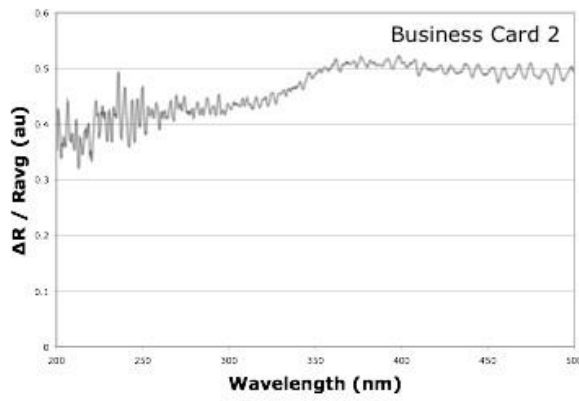


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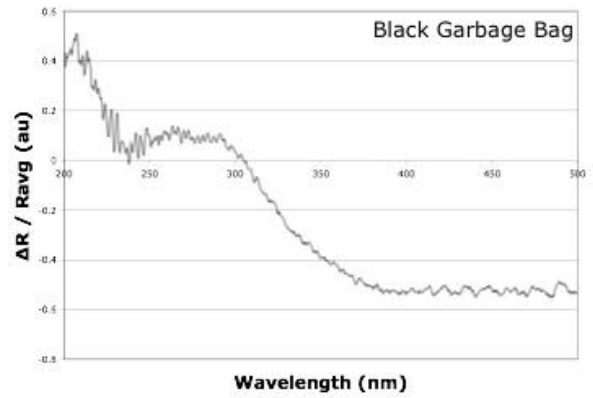


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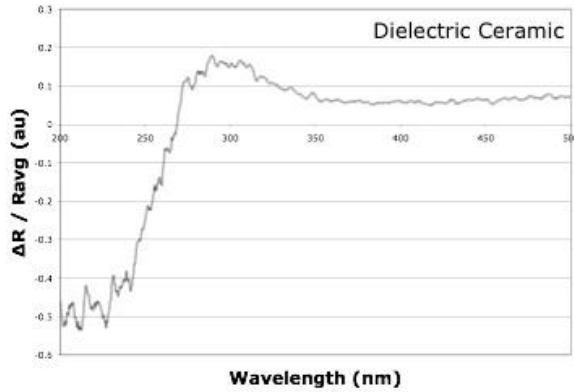


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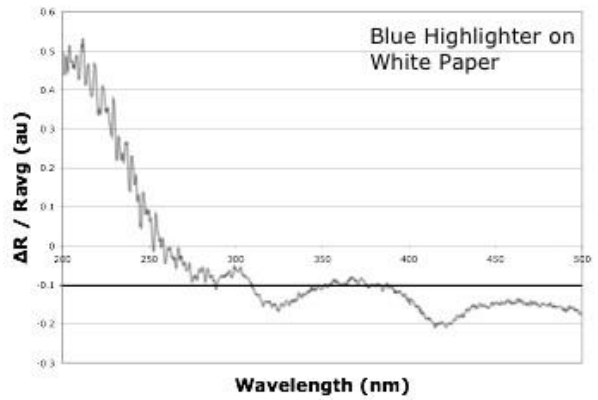


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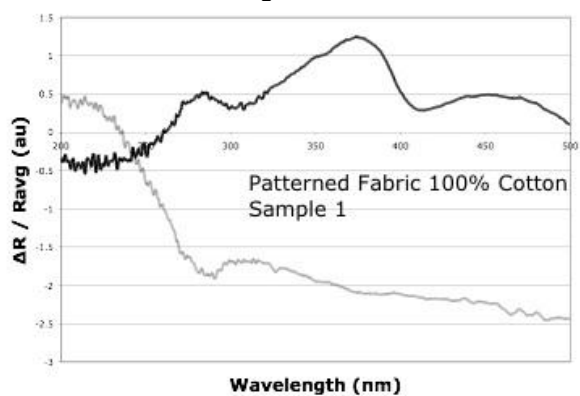


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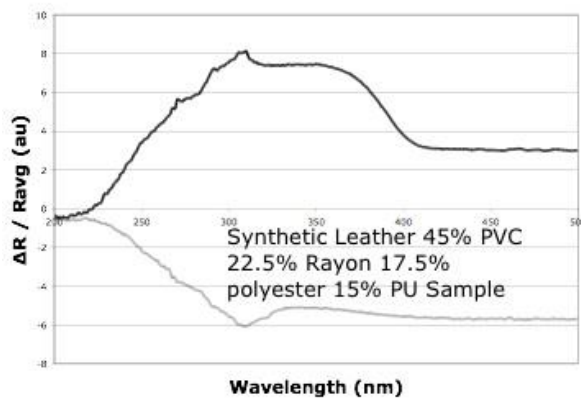


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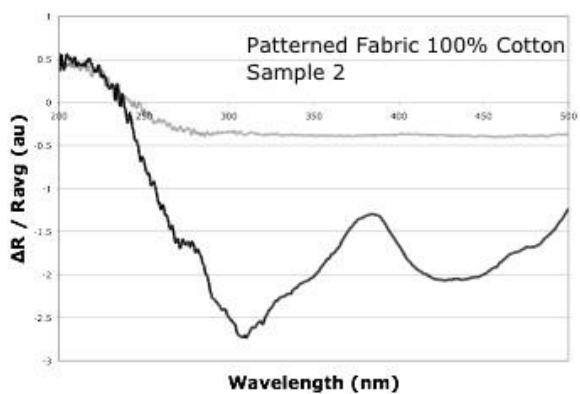


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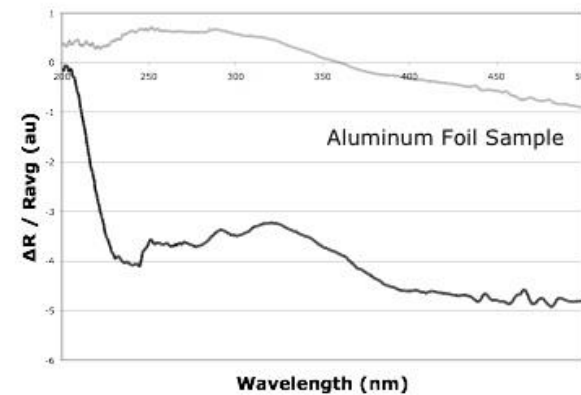


Figure 31

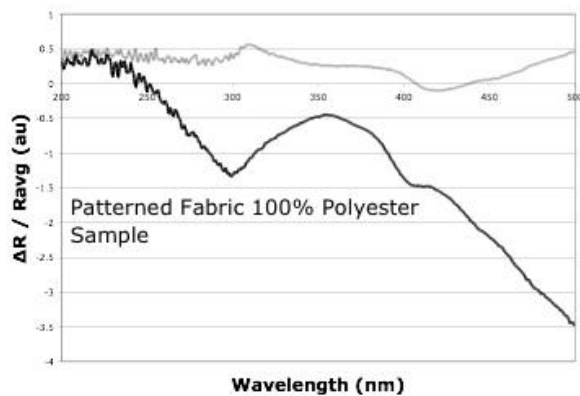


Figure 36: Comparison of samples tested with and without TNT present. Clockwise from top left: Particle board, Plywood 1, Pine Wood, Plywood 2. The darker lines are with TNT and the lighter lines are without TNT.

