

UNIVERSITY OF RHODE ISLAND

Department of Chemistry

Room 234 Pastore Hall

3:00 p.m, Monday, Feb. 22, 2016

Devon Swanson

Ph.D Research Seminar

Chemistry Department

URI

***“Intermolecular Interactions of
Energetic Materials”***

HOST

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Intermolecular Interactions of Energetic Materials

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A variety of intermolecular interactions occurs when an energetic material responds to its surroundings. With a better understanding of these energetic material contacts, improved performance on plastic-bonded explosives, superior swab materials for explosives detection, and novel insensitive munitions are possible. In that aim, the following relationships were examined: adhesion between energetic materials and polymer substrates; quantitative collection and detection of energetic materials on electrostatically charged swabs; and noncovalent derivative investigation between energetic material pairs.

Most explosive detection swab materials are burdened by either poor sorption (pickup) or poor desorption (release). Therefore, finding a swab that can both easily sorb and desorb an explosive is highly desirable. Atomic force microscopy, while typically employing a sharp (~5 nm) tip for topographic and force measurements, in this case was used to measure adhesion of energetic materials and candidate polymer swab materials. A micron-sized crystallite of energetic material was glued to a tipless cantilever, and force curve measurements were taken on flattened polymer substrates. While they indicate there are numerous polymers more adhesive than Teflon (a conventional explosives detection swab), the results do not reflect desorption capabilities.

Instead of using a new polymer swab or material, electrostatic charging of commercial off-the-shelf swabs was investigated as a method of increasing the attraction between the explosive and swab while retaining full desorption. Charging methods and conditions were tested, suggesting that humidity plays a large role in charge magnitude and retention.

In order to quantify explosive pickup on both contact and noncontact electrostatic swabs, a triple quadrupole liquid chromatograph/mass spectrometer was used. Chromatographic and mass spectral optimization were performed to lower the limit of detection to nanogram

quantities. A drop-on-demand printer was employed to dispense precise trace amounts of both explosive solutions and, to simulate real-world transfer, artificial fingerprint sebum.

The synthesis of the next generation of explosives is increasingly difficult as available novel reagents and synthetic techniques are limited. A recent approach to create new explosives is co-crystallization. Relying on noncovalent derivatives, cocrystals can tailor explosive properties, potentially yielding a new energetic material without novel molecule synthesis. Numerous energetic and non-energetic pairs were investigated for cocrystal potential, with few evidently successful results. Two pairs with intriguing results are nitrourea and 2,6-dinitrotoluene and trinitrotoluene and nicotinamide.