

UNIVERSITY OF RHODE ISLAND
Department of Chemistry PhD Seminar

Room 105 Beaupre
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**“The Effects of Positional Isomerization
on Energetic Materials”**

HOST
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The Effects of Positional Isomerization on Energetic Materials

Energetic materials are defined by the nature and high quantities of energy stored in the chemical bonds and ring strains of their molecules. Their high detonation velocities (e.g. RDX detonation velocity $[D_v] = 8806$ m/s), great thermal stability, and suitable sensitivities to initiation and handling are desirable features in applications such as mining, modern weapons and equipment development, and fireworks. Important considerations to acknowledge when working with an energetic material include verifying its sensitivity to ensure proper handling (e.g. TATP impact sensitivity $[IS] = 0.3$ J, too sensitive to unintentional detonation; RDX $[IS] = 7.5$ J, difficult to initiate) and knowing its storage life and density, which improves the detonation performance because there are more molecules (mass) that can react per unit volume. By accounting for these factors and considerations, the characterization of energetic materials is made possible based on their unique physicochemical properties (e.g. density and impact sensitivity). However, what if the physicochemical properties of energetic materials could be altered based on their positional isomers?

Evaluating the positional isomers of energetic materials would help researchers determine their physicochemical properties, which provide information on their effectiveness. Based on the applications of positional isomerism in other chemistry-related research fields such as drug isomerism in medicine, it can be surmised that positional isomerism has a role in the field of energetic materials. Performing an evaluation on the positional isomers of energetic materials would raise two questions: 1) is there a role for positional isomerism in energetic materials, and 2) how can their physicochemical properties be determined? In this talk, the physicochemical properties (density, impact sensitivity, and decomposition temperature) of two pairs of energetic isomers, 4-methylnitramino-1-methyl-3,5-dinitropyrazole (4-MMDNP) & 5-methylnitramino-1-methyl-3,4-dinitropyrazole (5-MMDNP) and 5,5'-bis(3,4-dinitro-1H-pyrazol-5-yl)-2H,2'H-3,3'-bi(1,2,3-triazole) (BDBT-1) & 5,5'-bis(3,5-dinitro-1H-pyrazol-4-yl)-1H,1'H-3,3'-bi(1,2,4-triazole) (BDBT-2), are evaluated using analytical instrumentation and mathematical methods such as differential scanning calorimetry (DSC) and the Kissinger method. The instrumental and mathematical methods' data obtained from each isomer in a pair provided insight on how their physicochemical properties could be fine-tuned, and how evaluating energetic isomers can help provide researchers with new energetic materials' design strategies.