

S&T Campaign: Sciences for Lethality and Protection

Kinetic Lethality

Effects on Target

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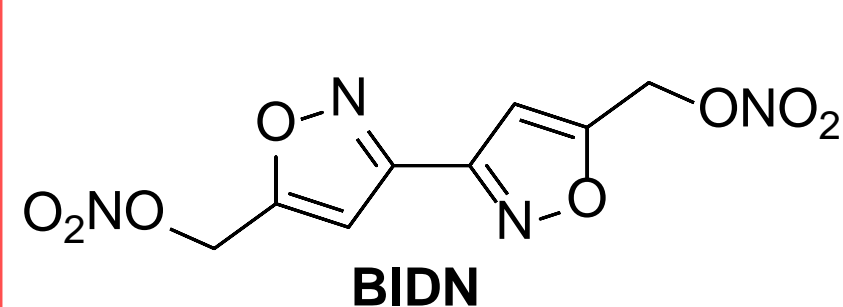
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Research Objective

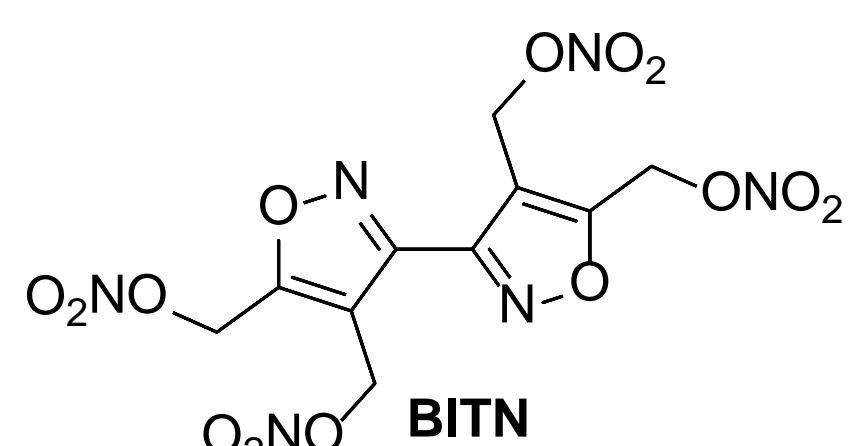
Develop novel energetic materials with reduced sensitivity for improved warhead effectiveness and for extended range propellants

Molecules Synthesized at ARL

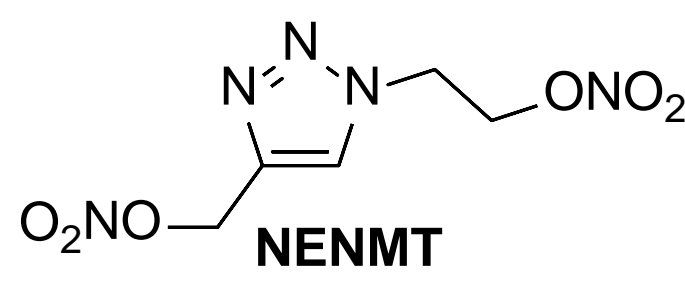
Energetic Plasticizer Ingredients



$T_{\text{melt}} = 96.2\text{ }^{\circ}\text{C}$
 $T_{\text{dec}} = 191.7\text{ }^{\circ}\text{C}$
 Density = 1.60 g/cc
 Heat of formation = -139 kJ/mol
 $P_{\text{cj}} = 19.3\text{ GPa}$
 $V_{\text{det}} = 7060\text{ m/s}$
 $I_{\text{sp}} = 206.2\text{ s}$

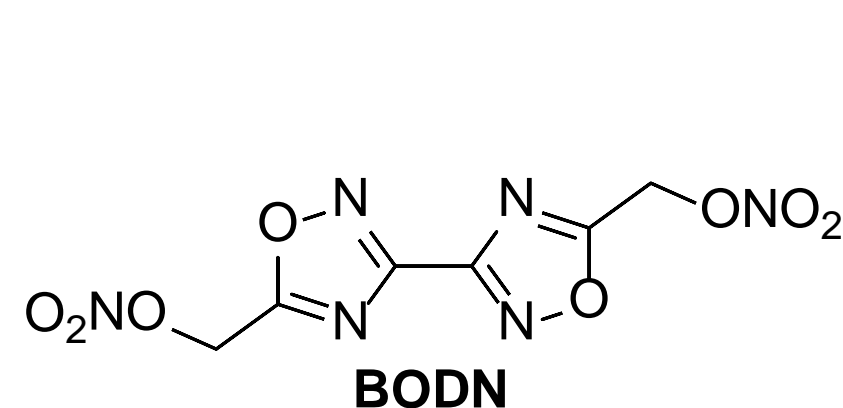


$T_{\text{melt}} = 125.0\text{ }^{\circ}\text{C}$
 $T_{\text{dec}} = 192.0\text{ }^{\circ}\text{C}$
 Density = 1.76 g/cc
 Heat of formation = -395 kJ/mol
 $P_{\text{cj}} = 25.6\text{ GPa}$
 $V_{\text{det}} = 7656\text{ m/s}$
 $I_{\text{sp}} = 236.0\text{ s}$

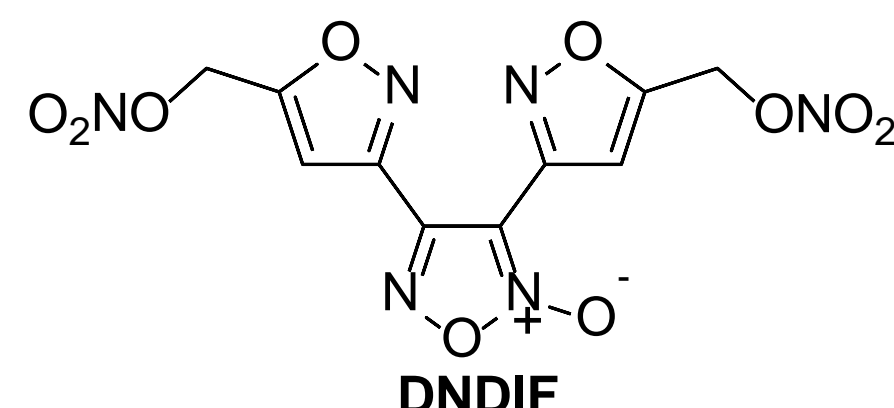


$T_{\text{dec}} = 128.0\text{ }^{\circ}\text{C}$
 Density = 1.60 g/cc
 Heat of formation = -39.1 kJ/mol
 $P_{\text{cj}} = 23.7\text{ GPa}$
 $V_{\text{det}} = 7468\text{ m/s}$
 $I_{\text{sp}} = 228\text{ s}$

Melt-Castable Explosive Ingredients



$T_{\text{melt}} = 82.0\text{ }^{\circ}\text{C}$
 $T_{\text{dec}} = 189.0\text{ }^{\circ}\text{C}$
 Density = 1.834 g/cc
 Heat of formation = -79.4 kJ/mol
 $P_{\text{cj}} = 29.4\text{ GPa}$
 $V_{\text{det}} = 8200\text{ m/s}$
 $I_{\text{sp}} = 236.0\text{ s}$



$T_{\text{melt}} = 90.0\text{ }^{\circ}\text{C}$
 $T_{\text{dec}} = 194.0\text{ }^{\circ}\text{C}$
 Density = 1.70 g/cc
 Heat of formation = +49.5 kJ/mol
 $P_{\text{cj}} = 25.1\text{ GPa}$
 $V_{\text{det}} = 7374\text{ m/s}$
 $I_{\text{sp}} = 221\text{ s}$

Research Strategy

- Seek advice from explosive and propellant formulators and theoreticians to identify capability gaps and specific needs
- Tailor our syntheses using this information to provide molecules of relevance that the energetics community wants
- If a new energetic has favorable properties, efforts are undertaken to make the process scalable
- Transition the energetic ingredient to explosive and/or formulators for further testing

ARL Facilities and Capabilities Available to Support Collaborative Research

- Small scale to pilot scale explosive synthesis capability
- Access to super computer clusters for modeling and simulation

Capabilities Sought in Collaboration

- Synthetic organic chemists for the synthesis of non-energetic scaffolds
- Expertise in stereochemical synthesis, heterocyclic synthesis, and catalytic methods

Peer-Reviewed Publications

1. E. C. Johnson, P. E. Guzmàn, L. A. Wingard, J. J. Sabatini*, R. A. Pesce-Rodriguez, "A Convenient and 'Greener' Synthesis of Methyl Nitroacetate," *ACS Organic Process Research & Development* **2017**, *21*, 1088-1090.
2. R. C. Sausa*, R. A. Pesce-Rodriguez, L. A. Wingard, P. E. Guzmàn, J. J. Sabatini, "Crystal structure of 3,3'-biisoxazole-5,5'-bis(methylene) dinitrate (BIDN)," *Acta Crystallographica Section E*, **2017**, *73*, 644-646.
3. L. A. Wingard, P. E. Guzmàn, E. C. Johnson, J. J. Sabatini*, G. W. Drake, E. F. C. Byrd, "Synthesis of bis-Isoxazole-bis-Methylene Dinitrate: A Potential Nitrate Plasticizer and Melt-Castable Energetic Material," *ChemPlusChem*, **2017**, *82*, 175-178.
4. L. A. Wingard, E. C. Johnson, P. E. Guzmàn, J. J. Sabatini*, G. W. Drake, E. F. C. Byrd, R. C. Sausa, "Synthesis of Biisoxazoletetrakis(methyl nitrate): A Potential Nitrate Plasticizer and Highly Explosive Material," *European Journal of Organic Chemistry*, **2017**, 1765-1768.
5. L. A. Wingard, P. E. Guzman, J. J. Sabatini*, "A Chlorine Gas-Free Synthesis of Dichloroglyoxime" *ACS Organic Process Research & Development*, **2016**, *20*, 1686-1688.