SHOCK17-2017-000443

Abstract for an Invited Paper
for the SHOCK17 Meeting of
the American Physical Society

**Synthesis of High-Energy CHNO Materials: Rational Design through Consultation with Formulators**[1]

JESSE SABATINI, US Army Research Laboratory

There is an ongoing quest to synthesize new energetic materials that have densities, detonation pressures, detonation velocities and specific impulses that are as high as possible. While this is a noble goal that should still be pursued, there is the tendency to overlook real world attributes required for potential applications. As such, many of the materials that are being synthesized, while perhaps garnering a lot of scientific press based on calculated performance, will not ultimately prove to be useful when formulated. In designing new CHNO ingredients, careful consideration of its final potential application allows the tailoring of syntheses in an effort to help meet pressing needs and to address capability gaps. Discussed will be the syntheses of several isoxazole- and 1,2,4-oxadiazole-based energetic materials, which were designed based on their promising attributes as compared to similar problematic heterocycles. These ring systems were carefully selected based on chemical intuition. The materials were prepared in high yields using simple processes, and displayed expectedly low sensitivities to impact, friction and electrostatic discharge. The calculated performances of these materials, and their potential applications will be discussed.

[1]The US Army is acknowledged for funding of this work.