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Manipulating explosive sensitivity through structural modifications in a nitrate ester system

VIRGINIA MANNER, Los Alamos Natl Lab

Understanding how condensed phase effects influence sensitivity is essential for developing next generation insensitive high explosives. However, the ability to predictably manipulate explosive sensitivity remains an elusive goal. Explosive sensitivity has been suggested to be governed by multiple factors, from intramolecular effects such as bond dissociation energy, oxygen balance, and the electrostatic potential of reactive functional groups, to larger scale effects, such as crystal structure and hot spot formation. We have developed derivatives of the explosive pentaerythritol tetranitrate (PETN) and examined them experimentally and theoretically, in order to better understand which properties influence sensitivity. With this molecular framework, we can evaluate how small changes to the structure of the molecule influence qualities such as oxygen balance, heat of formation, heat capacity, compressibility, crystal packing, and hydrogen bonding, through techniques such as differential scanning calorimetry, x-ray crystallography, and atomistic simulation. We have also used small-scale sensitivity testing as an initial tool to screen for large and consistent differences in handling sensitivity. We will discuss the many factors that contribute to sensitivity in this series of systematically-modified molecules as well as in existing well-studied explosive systems, such as triaminotrinitrobenzene (TATB) and nitroglycerin (NG).

In collaboration with: Thomas Myers, Marc Cawkwell, Edward Kober, Bryce Tappan, Geoffrey Brown, Mary Sandstrom, LOS ALAMOS NATL LAB.