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Tailoring the Sensitivity of Explosives via Elemental Substitution

VIRGINIA MANNER, DANIEL PRESTON, BRYCE TAPPAN, Los Alamos Natl Lab — PETN is a very common nitrate ester explosive that has been widely studied due to its use in military and commercial explosives. Recently, it was shown by Klapotke, et al. that the central carbon atom in PETN could be replaced with silicon, resulting in an extremely sensitive contact explosive. Calculations have shown that the central Si atom forms a strong bond with the oxygen of the nitro group in the intermediate step. This information can be used to tailor PETN into a less sensitive explosive. Derivatives of PETN have been prepared by substituting the central carbon atom with atoms such as phosphorous and nitrogen, since they form weak bonds with oxygen. With a fully characterized suite of PETN derivatives in hand, the sensitivity and performance properties of each material can be measured. We will discuss the sensitivity/performance properties of each derivative relative to its structure, and relate the new results to the previously calculated mechanism of decomposition of PETN. Derivatives of other common explosives will also be discussed.

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