Abstract Submitted
for the SHOCK09 Meeting of
The American Physical Society

Explanation of the Colossal Sensitivity of Silicon Pentaerythritol Tetranitrate (Si-PETN)[1] WEI-GUANG LIU, SERGEY ZYBIN, SIDDHARTH DASGUPTA, WILLIAM GODDARD III — A new extremely sensitive silicon-based explosive was recently synthesized in Germany by the nitration of tetrakis(hydroxymethyl)-silane, $Si(CH_2OH)_4$, with nitric acid. This silapentaerythritol tetranitrate (Si-PETN), $Si(CH_2ONO_2)_4$(tetrakis(nitratomethyl)-silane) has a molecular structure nearly identical to its carbon analog - PentaErythritol TetraNitrate (PETN), $C(CH_2ONO_2)_4$ - with the central carbon atom replaced by silicon. Unexpectedly, SiPETN shows dramatically increased sensitivity, exploding with just a touch of a spatula, making it extremely dangerous and difficult to study. We have performed DFT calculations on paths of unimolecular decomposition and identified a novel central carbon-oxygen (or silicon-oxygen) rearrangement which shows a dramatic difference that may explain the colossal sensitivity. In particular, this reaction in SiPETN has significantly lower barrier and far more exothermic, which leads to a large net energy release at very early stages of Si-PETN decomposition facilitating a fast temperature increase and expansion of the reaction zone.

[1]Supported by ARO and ONR

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Date submitted: 20 Feb 2009 Electronic form version 1.4