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Decomposition of Nitroplasticizer in Plastic Bonded Explosive **PBX 9501** DENISE PAULER¹, JOEL KRESS, Los Alamos National Laboratory — In the plastic bonded explosive PBX 9501, a 50/50 mixture of Estane 5703, a polyester urethane random copolymer, and nitroplastizer (NP) binds the HMX explosive crystals. Chemical kinetic mechanisms are being developed for the thermal degradation of NP for high temperatures (explosions) and low temperatures (natural and accelerated aging studies). The goal of this work is to investigate reaction mechanisms using density functional electronic structure theory in addition to the data obtained from explosion and aging experiments. NP consists of a 50/50 mixture of bis-2,2-dinitropropyl acetal and formal. Using 2,2-dinitro-1-methoxypropane as a model compound, a library of reactions was investigated to propose a mechanism for the decomposition of NP. The current mechanism begins with the elimination of HONO, which remains trapped within the material. HONO then adds onto the backbone of NP, which can lead to the formation of esters and oximes that may react further to produce carbon monoxide, carbon dioxide, and NO_x gases. This work is supported by the Enhanced Surveillance Campaign and the Advanced Simulation and Computing program.

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