

Abstract Submitted  
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**Initial Decomposition Mechanism study for the Energy Release from Electronical Excited Energetic Material** BING YUAN, Colorado State University — Decomposition of energetic materials FOX-7 and 3,4-dinitropyrazole (DNP) are investigated both theoretically and experimentally. The two energetic model systems 1-nitropyrazole and 4-nitropyrazole are also studied as a comparison for DNP. The NO molecule is observed as an initial decomposition product from all four materials subsequent to UV excitation and the observed NO products are rotationally cold ( $< 50$  K). The vibrational temperature of the NO product from DNP is 3300 K, 1400 K hotter than that of its model species. The vibrational temperature of the NO product from FOX-7 is 1900 K. The initial decomposition mechanisms of these materials are explored at the complete active space self-consistent field (CASSCF) level. Potential energy surface (PES) calculations at the CASSCF(12,8)/6-31+G(d) level illustrate that conical intersections play an essential role in the decomposition mechanism. Electronically excited S2 molecules can nonradiatively relax to lower electronic states through (S2/S1)CI and (S1/S0)CI conical intersections and undergo a nitro-nitrite isomerization to generate an NO product either on the S1 state or S0 state PES. For model systems, NO is generated on the S1 state PES, while for the energetic materials FOX-7 and DNP, NO is produced on the ground state PES,

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