

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Comparison of Electronically Excited Photodissociation between Nitramine Energetic Materials and Model Systems YUANQING GUO, MARGO GREENFIELD, ATANU BHATTACHARYA, ELLIOT BERNSTEIN, Department of Chemistry, Colorado State University — Nitramine energetic materials (RDX, HMX and CL20) have broad applications as explosives and fuels. Model systems (1,4-dinitropiperazine, nitropiperidine, nitropyrrolidine and DMNA) have similar molecular structures, but they are unable to be used as fuels and explosives. To elucidate the difference between them, both nanosecond and femtosecond mass resolved excitation spectroscopy have been employed to investigate the mechanisms and dynamics of the electronically excited photodissociation of these materials. NO is a dominant dissociation product. Based upon the experimental observation and calculations of potential energy surfaces for these systems, we suggest that energetic materials dissociate from their ground electronic states after relaxing from the first excited states, and that the model systems dissociate from their excited state. In both cases a nitro-nitrite isomerization is part of the reaction mechanism. Parent ions of DMNA and nitropyrrolidine are observed in fs experiments. All the other molecules generate NO as a product even in fs time regime.

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Date submitted: 20 Nov 2006

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