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Quantum Chemical Studies on the Photochemistry of Nitro-Aromatic Explosives JASON QUENNEVILLE, Spectral Sciences, Inc., MARGO GREENFIELD, DAVID S. MOORE, Los Alamos National Laboratory — The use of temporally and spectrally shaped ultrafast laser pulses to initiate, as well as detect, high explosives is being explored at Los Alamos. High level quantum chemical calculations, presented here, provide vital support for this effort. Among the most widely-used high explosives are nitro-substituted benzene compounds such as 2,4,6-trinitrotoluene (TNT). The ground and excited electronic state potential energy surfaces of TNT and two other nitroarenes, nitrobenzene and 2,4,6trinitroaniline (TNA) have been investigated using multi-configurational ab initio and time-dependent DFT methods. We will describe the electronic absorption spectra as well as the geometrical and energetic character of the excited state reaction coordinates and conical intersections in the three compounds. The mechanisms for radiative and non-radiative quenching of excited state population, and possibilities for control will be outlined. The photochemistries of the three compounds are compared so that general statements on the photochemistry nitro-aromatic explosives can be made.

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