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Nature of electronic excitations in pentaerythritol tetranitrate crystals doped with 9,10-phenanthrenequinone¹ GUZEL GARIFZIANOVA, Kazan National Research Technological University, ROMAN TSYSHEVSKIY, University of Maryland College Park, ANTON ZVEREV, ANATOLY MITROFANOV, Kemerovo State University, MAIJA KUKLJA, University of Maryland College Park — Electronic properties, optical absorption and chemical reactivity of organic ketones and quinone molecules have been widely studied because of their ability to abstract hydrogen atoms from other organic molecules once excited to the highly reactive $^3(n,\pi^*)$ state. Most of these studies were done for liquid solutions. In this joint theoretical and experimental study, we focused on excited states of pentaerythritol tetranitrate (PETN) crystals doped with 9,10-phenanthrenequinone (PQ) molecules. We explored electronic properties of the system and estimated energies of the electronic excitations. It was found that PQ molecule in its excited triplet state can catalyze unusual decomposition pathways of PETN, which are not attainable through the potential surface of the ground state. We discuss mechanisms of such autocatalytic reactions in PETN-PQ complexes.

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