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Hydrogen transfer in energetic materials from ReaxFF and DFT calculations OLEG SERGEEV, ALEXEY YANILKIN, Dukhov All-Russia Research Institute of Automatics (VNIIA) — Reactive molecular dynamics is a tool enabling studies of thermal decomposition of explosives at realistic time scales. In the present work we construct a kinetic model of thermal decomposition of isolated molecules and condensed phase of PETN using results of ReaxFF simulations. The obtained parameters indicate that the activation energy is lowered by 50 kJ/mol in condensed phase compared to the unimolecular decomposition. The governing process in condensed phase decomposition proves out to be the intermolecular hydrogen transfer. The intra- and intermolecular hydrogen transfer is studied in detail with nudged elastic band technique in both ReaxFF and DFT descriptions. Two simpler energetic materials, nitrotoluene and methyl nitrate, are chosen for these calculations to lower the computational cost in DFT. In both materials ReaxFF gives the activation barrier for the intermolecular hydrogen transfer about 100 kJ/mol lower than that in DFT calculations. This may influence the applicability of ReaxFF in kinetics-related simulations of explosives. Computation protocol applied in this work may be used to systematically improve reactive potential for better description of chemical kinetics.

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