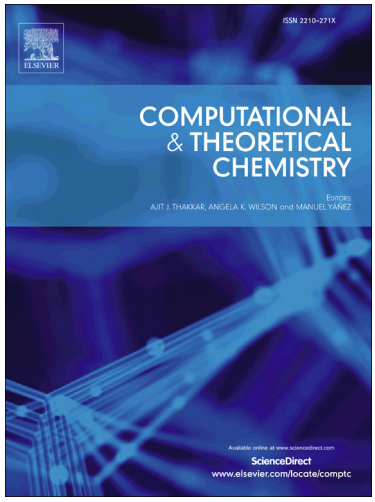

Theoretical investigation into the influence of molar ratio on binding energy, mechanical property and detonation performance of 1,3,5,7-tetranitro-1,3,5,7-tetrazacyclo octane (HMX)/1-methyl-4,5-dinitroimidazole (MDNI) cocrystal explosive

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Abstract

Molecular dynamics (MD) method was performed to study the effects of molar ratios on the structures and properties of 1,3,5,7-tetranitro-1,3,5,7-tetrazacyclo octane (HMX)/1-methyl-4,5-dinitroimidazole (MDNI) cocrystal explosives. The N–NO_2 trigger bond and surface electrostatic potentials were studied by the B3LYP method. Detonation properties of 1:1 HMX/MDNI cocrystal were calculated. The results show HMX/MDNI prefers cocrystalizing at the molar ratio of 1:1, at which the binding energy of extended model is the largest and the elastic modulus is the smallest among all the molar ratios (including pure HMX). Meanwhile, the poisson's ratio and *K*/*G* values of all the extended models are larger than those of HMX. $C_{12}-C_{44}$ of all the extended models, especially the 1:1 model, are larger than pure HMX, indicating the comprehensive mechanical properties may present at 1:1. Radial distribution function shows stronger non-bonded interaction may appear at 1:1 or 4:3. The structure and N–NO_2 bond analyses indicate that the sensitivity change of HMX/MDNI cocrystal explosive derives from not only the formation of hydrogen bonds, but also the reinforcement of N–NO_2 bonds. The detonation performances of HMX/MDNI suggest that the HMX/MDNI cocrystal possesses high power and low sensitivity.

Keywords: Co-crystal; Molecular ratios; MDNI; Molecular dynamics simulation; Density functional theory.

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