457. Title:Preparation and characterization of a novel cocrystal explosive
Authors:Shen, Jin P. (1); Duan, Xiao H. (1); Luo, Qing P. (1); Zhou, Yong (2); Bao, Qiaoliang (3); Ma, Yong J. (1); Pei, Chong H. (1)
Source title:Crystal Growth and Design
Volume:11
Issue:5
Issue date:May 4, 2011
Publication year:2011
Pages:1759-1765
Language:English
Document type:Journal article (JA)
Abstract:On the basis of our previous Molecular Dynamics (MD) Simulation (Wei, C. X.; Huang, H.; Duan, X. H.; Pei C. H. Propell. Explos. Pyrot. 2009, 67, 2822-2826), a cocrystal explosive (CCE) consisting of octahydro-1,3,5,7- tetranitro-1,3,5,7-tetrazocine (HMX) and 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) has been prepared with a solvent/nonsolvent (S/NS) process. Scanning electron microscopy (SEM) demonstrated that crystal morphology of the CCE was significantly improved in contrast to the crystal of HMX and TATB. Differential scanning calorimetry (DSC) showed that the CCE exhibited the enhancement of thermal stability and became less sensitive to impact, compared with the HMX. Raman spectroscopy, terahertz time-domain spectroscopy (THz-TDS), and X-ray photoelectron spectroscopy (XPS) provided characterization at the molecular level. The results indicated that the main mechanism of cocrystal originates from the N-O &middot &middot &middot H hydrogen bonding between-NO 2 (HMX) and-NH2 (TATB).