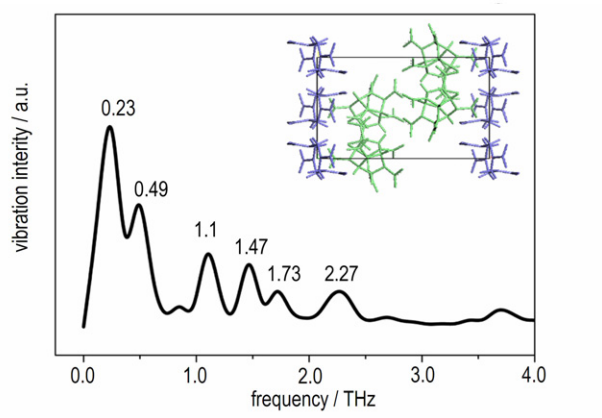
Theoretical Studies for THz Spectra of CL-20/HMX Cocrystal

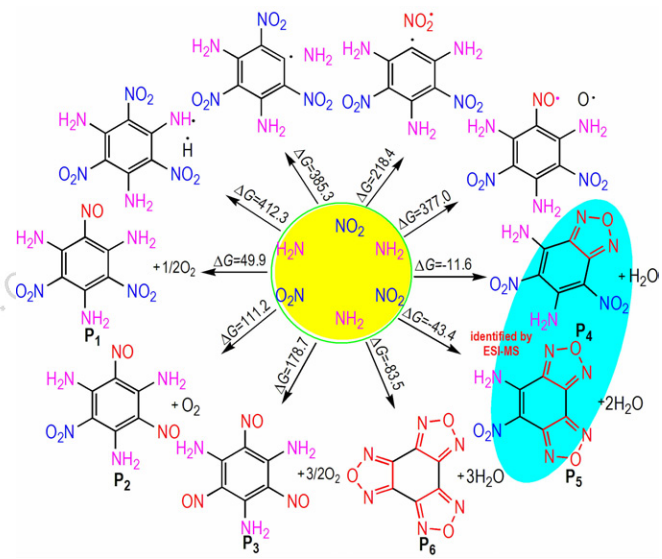


AN Qing, DUAN Xiao-hui, SHI Lu, PEI Chong-hua

Chinese Journal of Energetic Materials, 2017, 25(7): 533–539

Taking hexanitrohexaazaisowurtzitane (CL-20)/cyclotetramethylenetetranitramine (HMX) cocrystal as the model system, the THz spectra of cocrystal components β-HMX, CL-20, and CL-20/HMX cocrystal were theoretically studied by combining the methods of molecular dynamics simulation and quantum mechanics. The assignment and analysis of vibration modes for characteristic peaks were carried out. The response of different intermolecular interactions in THz spectra was confirmed.

Mechanism of Radiation-induced Colour Change in 1,3,5-Triamino-2,4,6-trinitrobenzene under γ-Rays

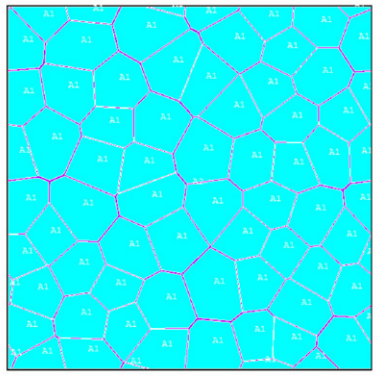


AO Yin-yong, CHEN Jie, SONG Hong-tao, SHI Jian-min, LIU Yu, CHEN Hong-bing, LI Jiu-qiang, PENG Jing

Chinese Journal of Energetic Materials, 2017, 25(7): 540–545

The thermodynamic parameters and the excited states ofradiolysis products of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) were obtained by density functional theory calculation (DFT). The gamma-ray radiolysis products of TATB were studied by high-resolution electrospray ionization mass spectrometry (ESI-MS).

Predicting the Effective Elastic Modulus of PBX Based on Voronoi Meso-scale Numerical Model

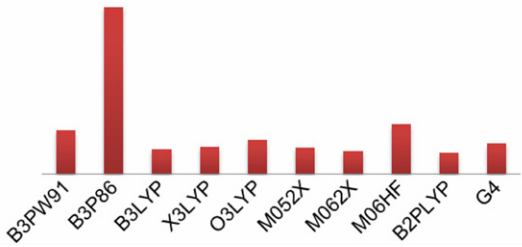


Periodic representative volume element models were established to predict the effective elastic modulus of PBX. According to the meso-structure of polymer bonded explosives (PBX), irregular polygonal particle models based on Voronoi method were established, which achieved extremely high particle volume fraction (over 85%).

WANG Jing-cheng, LUO Jing-run

Chinese Journal of Energetic Materials, 2017, 25(7): 546–551

Theoretical Investigations on Fundamental Performances of All-nitrogen Materials: Ⅱ. Prediction of Enthalpies of Formation

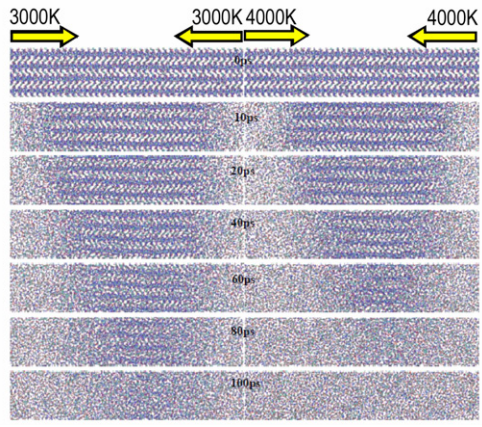


LIU Ying-zhe, LAI Wei-peng, YU Tao, GE Zhong-xue, LUO Yan-jiao, XU Tao, YIN Shi-wei

The enthalpies of formation of 52 nitrogen-rich compounds were calculated by different density functionals.

Chinese Journal of Energetic Materials, 2017, 25(7): 552–556

Reactive Flow Propagation in CL-20/TNT Co-crystal Explosive Induced by Local High Temperature Zones: ReaxFF Molecular Dynamics Simulations

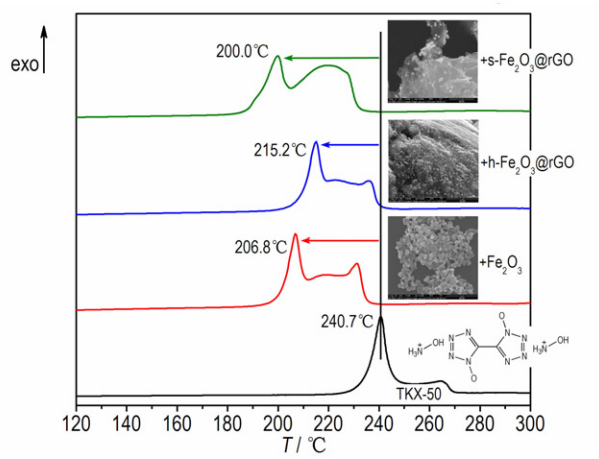


In order to better understand the phenomenon and mechanism of thermal ignition and hot spots growth in energetic materials, two kinds of high temperature conditions (3000 K, 4000 K) are applied to two ends of CL-20/TNT co-crystal and keeping it combining NVT ensemble and Berendsen temperature coupling method. High temperature induced reactive flow propagation and chemical reaction details are studied by ReaxFF reactive force field molecular dynamics simulations.

LIU Hai, YANG Zhen, HE Yuan-hang

Chinese Journal of Energetic Materials, 2017, 25(7): 557–563

Preparation of Fe_2O_3@rGO Nanocomposites and Their Effect on the Thermal Decomposition of TKX-50

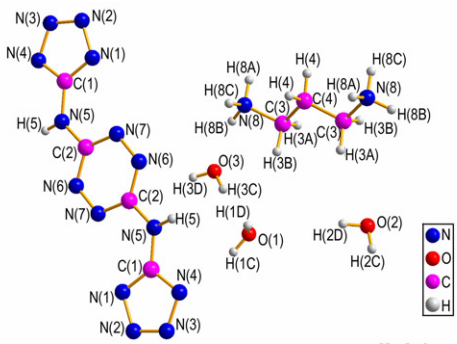


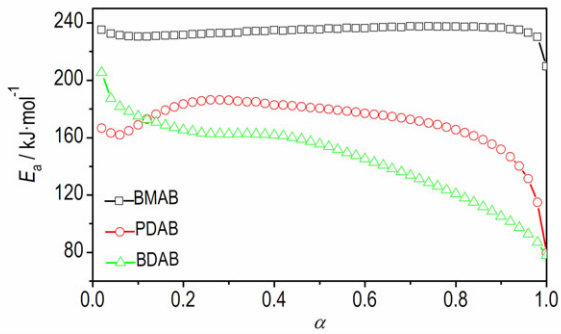
ZHANG Jian-kan, ZHAO Feng-qi, XU Si-yu, YANG Yan-jing, QU Wen-gang

Chinese Journal of Energetic Materials, 2017, 25(7): 564-569

h-Fe_2O_3@rGO and s-Fe_2O_3@rGO nanocomposite was prepared using hydrothermal and solvothermal method, respectively, and as an effective catalyst for the decomposition of TKX-50.

Synthesis and Properties of Energetic Ionic salts Based on 3,6-Bis(1*H*-1,2,3,4-tetrazol-5-yl-amino)-*s*-tetrazine(BTATz)



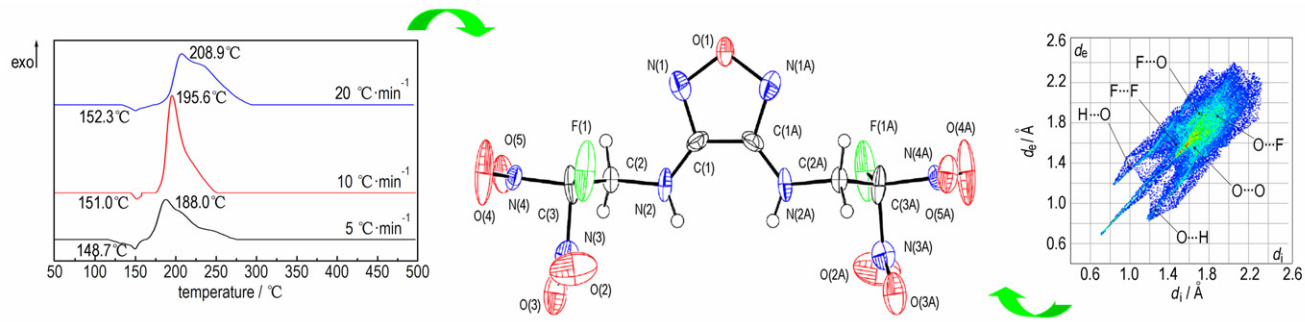


LIU Qing, YANG Jin, REN Ying-hui, MA Hai-xia, XU Kang-zhen, ZHANG Chao, ZHAO Feng-qi, HU Rong-zu

Chinese Journal of Energetic Materials, 2017, 25(7): 570-578

Three energetic salts based 3,6-bis(1*H*-1,2,3,4-tetrazol-5-yl-amino)-*s*-tetrazine(BTATz), DMAB, PDAB and PDAB were prepared and the crystal structure of 1,3-propanediamine salt was determined. The main thermal decomposition kinetic mechanisms of the three salts were obtained with non-isothermal method.

Crystal Structure and Thermal Properties of *N*, *N*′-Bis (2-fluoro-2,2′-dinitroethyl)-3,4-diaminofurazan

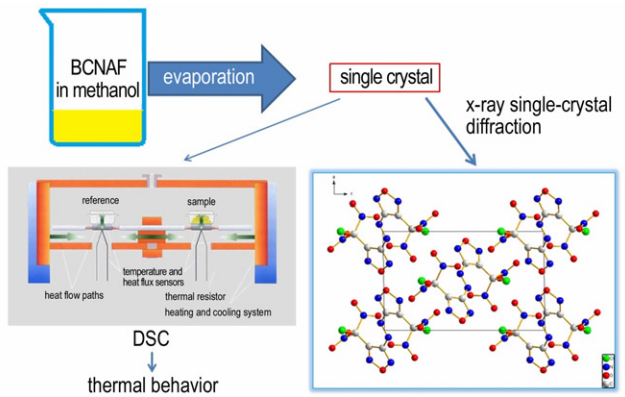


MA Qing, LU Huan-chang, LIAO Long-yu, HUANG Jing-lun, FAN Gui-juan, LIU Yong-gang

***Chinese Journal of Energetic Materials*,2017,25(7):579–584**

The single-crystal of *N*,*N*′-bis(2-fluoro-2,2′-dinitroethyl)-3,4-diaminofurazan (LLM-208) was obtained for the first time. Its crystalline properties, intermolecular interaction in moleular crystal and thermal decomposition performance were further investigated.

Crystal Structure and Thermal Stability of 4,4′-Bis (chlorodinitromethyl)-3,3′-azofurazan

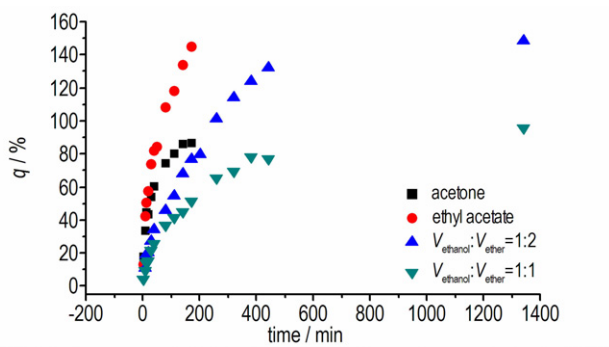


GU Hao, MA Qing, YANG Hong-wei, CHENG Guang-bin, FAN Gui-juan

***Chinese Journal of Energetic Materials*,2017,25(7):585–590**

A new energetic compound 4,4′-bis(chlorodinitromethyl)-3,3′-azofurazan was synthesized as an important intermediate. Its structure was firstly confirmed by X-ray single-crystal diffraction. The thermal stability was determined by thermo-gravimetric analysis(TG) and differential scanning calorimetry(DSC).

Swelling Behaviors of NC/NG Absorbent Tablets

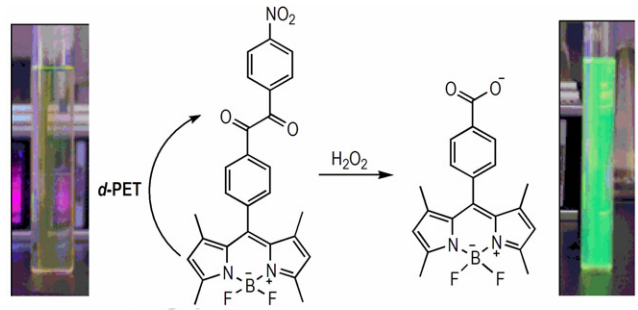


WANG Qiong, DENG Chong-qing, WEI Hong-jian, LI Ji-zhen, ZHANG Lin-jun

***Chinese Journal of Energetic Materials*,2017,25(7):591–596**

The free swelling process of absorbent tablet with or without predrying treatment in solvents was studied using the weighting method.

Novel Fluorescent Probe Based on BODIPY for the Detection of Hydrogen Peroxide

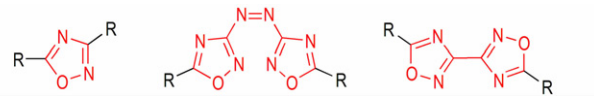


LI Bao-sheng, CHEN Jian-bo, SUN Jie

Chinese Journal of Energetic Materials,2017,25(7): 597–602

A novel fluorescent probe 4-(4-nitro-benzyl)-boron-dipyrromethene (BD-3) was designed and synthesized by using benzyl as the recognition group and boron-dipyrromethene (BODIPY) as the fluorophore. The chemical structure of BD-3 was characterized and its detection performance was investigated to meet the requirement of on-site detection of peroxide explosives under complex environmental conditions.

Review on Energetic Compounds Based on 1,2,4-Oxadiazoles

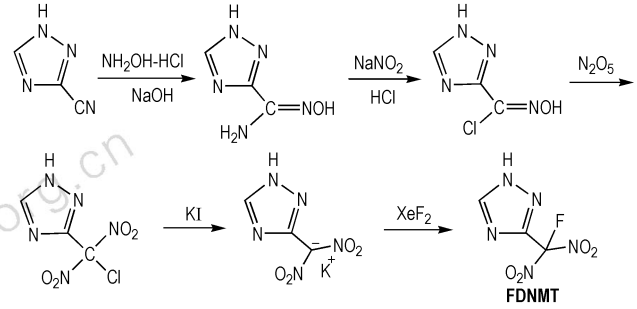


HUANG Xiao-chuan, WANG Zi-jun, GUO Tao, QIN Ming-na, LIU Min, QIU Shao-jun

Chinese Journal of Energetic Materials,2017,25(7): 603–611

In this paper, the latest research achievements of more than 30 oxadiazole energetic compounds base on mono-1,2,4-oxadiazoles, azo-1,2,4-oxadiazoles and bis-1,2,4-oxadiazoles were reviewed.

Synthesis and Properties of 3-Fluorodinitromethyl-1,2,4-triazole



LI Ya-nan, SHU Yuan-jie, ZHANG Sheng-yong, WANG Bo-zhou, ZHAI Lian-jie, HUO Huan

Chinese Journal of Energetic Materials,2017,25(7): 612–616

3-Fluorodinitromethyl-1,2,4-triazole (FDNMT) was synthesized using 3-cyano-1,2,4-triazole as starting material. The structure of FDNMT was confirmed by IR, ^{1}H NMR, ^{13}C NMR, elemental analysis and MS. The single crystal of FDNMT was obtained in the acetonitrile system. The detonation properties of FDNMT were calculated using Gaussian 09 program and Kamlet-Jacobs equations.