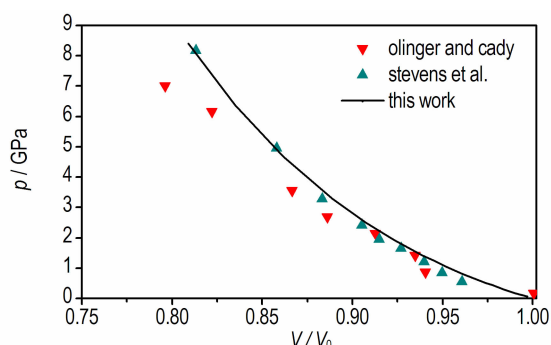


Density Functional Theory Study on Equation of State and Vibration Properties of TATB Crystal

JIANG Wen-can, CHEN Hua, ZHANG Wei-bin

Chinese Journal of Energetic Materials, 2016, 24(7): 625–631

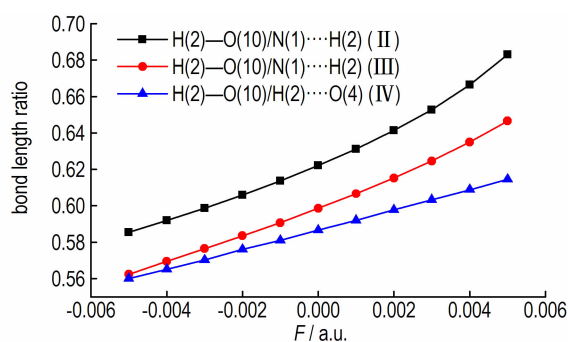


Non-local van der Waals correction was used to calculate the equation of state of TATB crystal. The result was found to be in good agreement with the experiment data. Based on the calculated results, the equation of state and vibration properties of TATB crystal at pressure of 0 GPa to 8.5 GPa were studied. The vibration modes were re-assigned. Mode coupling and intermolecular interaction were analyzed.

Density Functional Theory Study on the Influence of Electric Field on Hydroxylamine Nitrate

LIU Jian-guo, ZHANG Qian, AN Zhen-tao, ZHEN Jian-wei, WANG Chao-yang

Chinese Journal of Energetic Materials, 2016, 24(7): 632–638

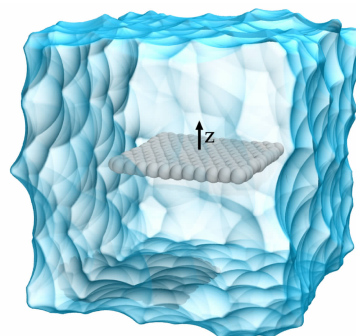


Three fully optimized geometries of hydroxylamine nitrate ion pair have been obtained with density functional theory method at the B3LYP/6-311++G(d, p) level without the electric field. Natural bond orbital analysis was performed to reveal the origin of the interaction. Bond length, binding energy and level distribution under different electric fields ranging from -0.005 a. u. to 0.005 a. u. were calculated.

Structural Arrangements of Nitromethane on the Graphene Surface

LIU Ying-zhe, LAI Wei-peng, WANG Yu, YU Tao, REN Gan, GE Zhong-xue, KANG Ying

Chinese Journal of Energetic Materials, 2016, 24(7): 639–643

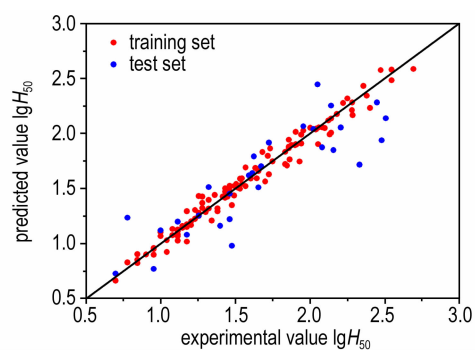


The structural arrangements of nitromethane on the graphene surface were investigated by the analysis of interaction energies, density distribution, dipole orientation, and ordering effect obtained from molecular dynamics simulations.

Prediction of Impact Sensitivity of Polynitro Compounds by Artificial Neural Network Based on the Genetic Algorithm

QIAN Bo-wen, CHEN Li-ping, CHEN Wang-hua

Chinese Journal of Energetic Materials, 2016, 24(7): 644–650

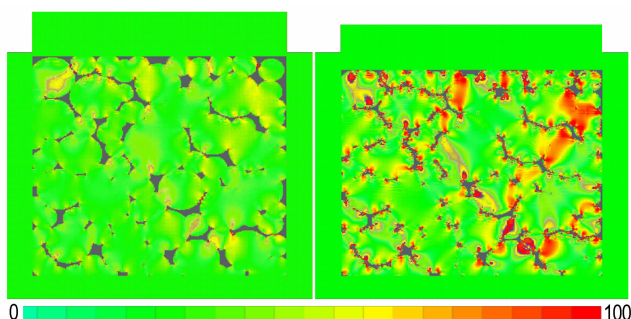


Based on QSPR principle, the quantitative relationship between impact sensitivity and molecular structures of polynitro compounds was investigated by multiple linear regression (MLR) and artificial neural network (ANN) using the molecular descriptors got by genetic algorithm.

Two Dimensional Numerical Simulation for Mesoscopic Mechanics Behaviors of PBX in Pressing Processes

TANG Hong, ZHOU Jun-hui, Lü Ke-zhen, CHEN Xue-ping, DOU Yu-sheng

Chinese Journal of Energetic Materials, 2016, 24(7): 651–656

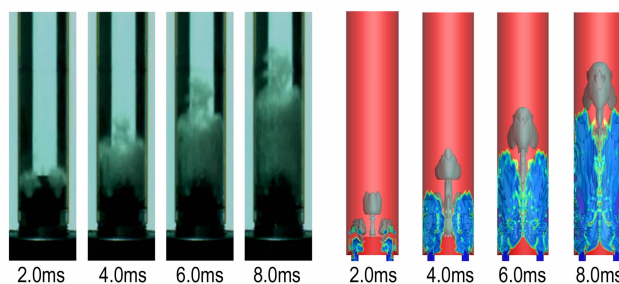


Mechanics behaviors and temperature of PBX in pressing process have been simulated by the material point method.

Influence of Injection Structure on Gas-curtain Generation Characteristics in Liquid Tube by Numerical Analysis

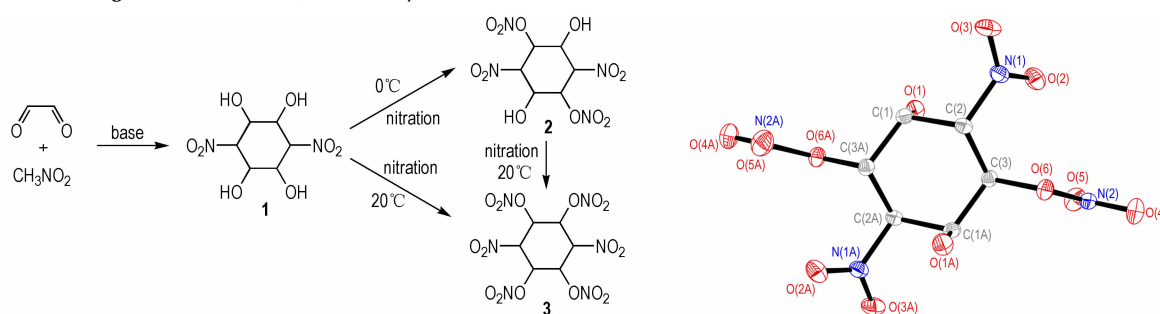
ZHOU Liang-liang, YU Yong-gang, CAO Yong-jie

Chinese Journal of Energetic Materials, 2016, 24(7): 657–663



Three-dimensional unsteady mathematical model of multi gas jets in liquid tube was established to research the influence of injection structure on gas-curtain generated by underwater launched gun. The distribution of phase, pressure and velocity were numerical acquired.

Synthesis, Crystal Structure and Thermal Properties of Two Nitrate Ester Energetic Materials of 3,6-Dinitrocyclohexane

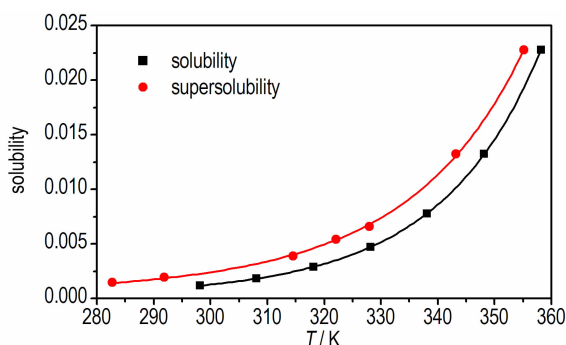


Two nitrate ester energetic materials 1,4-dihydroxy-2,5-dinitro-3,6-dinitrocyclohexane (**2**) and 1,2,4,5-tetranitro-3,6-dinitrocyclohexane (**3**) were synthesized from glyoxal and nitromethane by condensation and nitration, and the structures were characterized by IR, NMR, and elemental analysis.

LI Xiang-zhi, LI Hui, LIAN Peng, LAI Wei-peng, ZHOU Cheng, WANG Bo-zhou

Chinese Journal of Energetic Materials, 2016, 24(7): 664–668

Cooling Crystallization Kinetics of 3,4-Bis(3-nitrofurazan-4-yl) furoxan

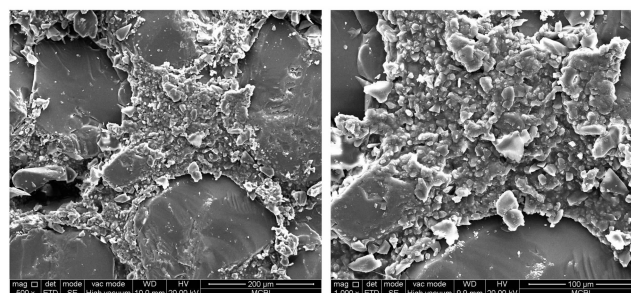


The solubility, supersolubility and cooling crystallization kinetics of 3,4-bis(3-nitrofurazan-4-yl) furoxan (DNTF) in V(acetic acid) : V(water) = 7 : 3 mixed solvent were studied by a batch crystallizer. The nucleation and growth rate equation of DNTF cooling crystallization were determined.

HOU Huan, WANG Jian-long, CAO Duan-lin, ZHOU Yan-shui, CHEN Li-zhen, LAN Guan-chao

Chinese Journal of Energetic Materials, 2016, 24(7): 669–673

Aging Damage and Mechanical Environment Adaptability of Pressed HMX-Based PBX

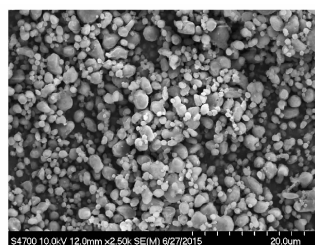


The natural storage method was carried out to investigate the aging damage of pressing HMX-based PBX. The aging defects of the charge structures stored for 4, 8 and 12 years were observed by CT scanning, and the charge micro morphology stored for 4 and 12 years were characterized by SEM. The mechanical environment adaptability stored for 12 years was evaluated by impact and vibration test.

YIN Jun-ting, YUAN Bao-hui, SHI Wei-wei, WANG Jian-chao, GAO Yu-ling

Chinese Journal of Energetic Materials, 2016, 24(7): 674–677

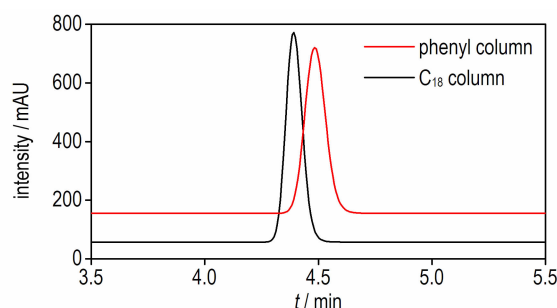
Design of Nozzle Structure for SEDS Technology to Prepare Sub-micron RDX Particles



A new type of nozzle for solution enhanced dispersion by supercritical fluids (SEDS) was designed, and the effect of nozzle structure on the preparation of ultrafine RDX was analyzed, and the most reasonable structure design of nozzle was obtained. An average particle size 660 nm, distribution range of 0.1 ~ 2 μm , spherical, submicron particles RDX are prepared.

CAI Xing-wang, YANG Ji-hua, ZHANG Jing-lin, XU Hong-yan
Chinese Journal of Energetic Materials, 2016, 24(7) : 678–685

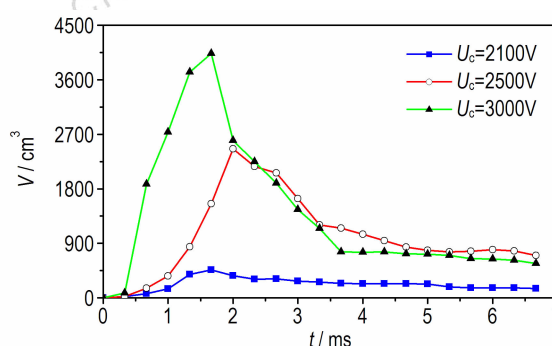
Determination of PETN Content in PBX by High Performance Liquid Chromatography



A selective and sensitive high performance liquid chromatography (HPLC) was optimized for quantitative analysis of pentaerythritol tetranitrate (PETN) based polymer bonder explosive (PBX). The influences of sample treat method, sample mass and solvent were studied.

CHEN Ling, PANG Xiao-qing, ZHAO Ying-bin, ZHANG Yong
Chinese Journal of Energetic Materials, 2016, 24(7) : 686–691

Measurement and Analysis of the Expansion Characteristics of Pulsed Plasma Jet in Air



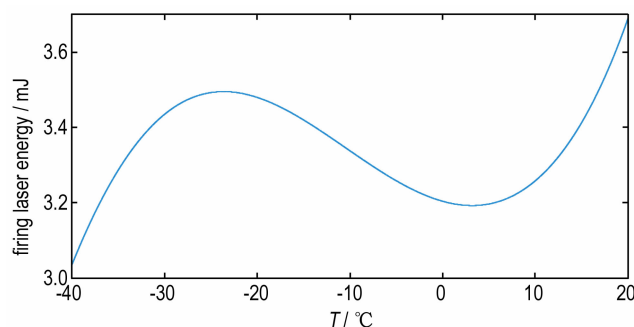
The expansion process of pulsed plasma jet generated by a plasma generator was studied by a piezoelectric pressure sensor and a digital high-speed video system. The relation of change in the extended volume, axial displacement and radial displacement of pulsed plasma jet in atmosphere with time under different discharge voltage and jet breaking pressure was treated and obtained by Photoshop etc software.

ZHAO Xue-wei, YU Yong-gang, MANG Shan-shan
Chinese Journal of Energetic Materials, 2016, 24(7) : 692–697

Influence of Low Temperature on Laser Transmission Efficiency in Laser Initiation Subsystem

HE Ai-feng, CHU En-yi, CAO Chun-qiang, JING Bo, XU Feng-yi, LI Ming, ZHAO Dong-ya

Chinese Journal of Energetic Materials, 2016, 24(7): 698–702

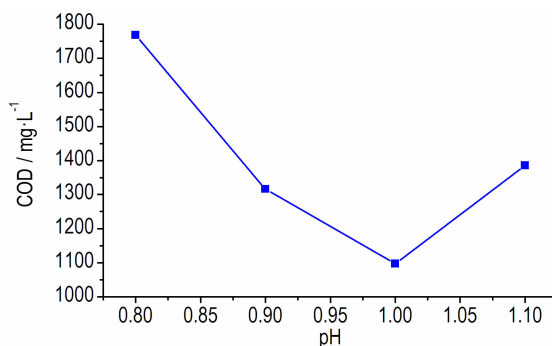


To evaluate the reliability of laser diode initiation (LDI) subsystem at low temperature (−40–20 °C), the performance of a dual-way LDI subsystem and its individual parts was studied by environmental test and initiation test. The minimum delivered firing energy to each laser initiator was calculated with fitting experiential formula, the total margin factor of the LDI subsystem was calculated.

Pretreatment of TNT Red Water by Complex Extraction

WANG Qian, ZHANG Yan-wen, LI Ming, YIN Hong-quan, MA Ru-yi, YANG Xin-tao, CHEN Fu-xue, WU Yu-kai

Chinese Journal of Energetic Materials, 2016, 24(7): 703–708

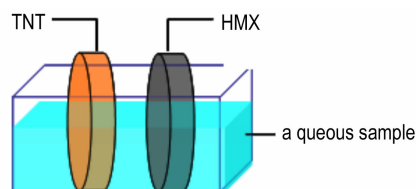


The TNT red water in the process of TNT production was pretreated by the complex extraction using trinoctylamine as a complex extraction agent. The effect of pH value, stirring speed, stirring time and the ratio of the extraction agent and the wastewater on the extraction efficiency was studied.

Reuse of Wastewater in Explosive Machining Process with Ceramic Ultra-filtration Membranes

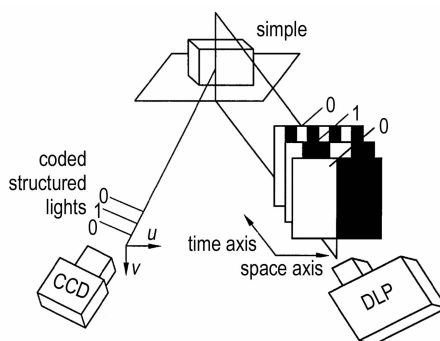
LI Shi-chun, LIU Yu, YIN Rui, LUO Li-yuan, QING Hou-qing, XU Rui-juan

Chinese Journal of Energetic Materials, 2016, 24(7): 709–714



Ceramic ultra-filtration membranes could be used to remove the suspended solids for the reuse of explosive wastewater. The effects of operation parameters on permeate flux and turbidity were investigated. The membrane fouling was investigated by concentration and washing experiments. Moreover, the water quality analysis and explosive column immersing experiments were proposed to investigate the feasibility for reuse of wastewater.

Application Progress of Geometrical Parameters Measurement Techniques for Energetic Materials Component



The current research on measuring technology with mechanical device, coordinate measuring techniques, portable coordinate measuring techniques and 3D optical no-touching measurement techniques for the energetic materials component at home and abroad were summarized.

LIU Yong, GAO Guo-fang, ZHANG Xiao-hua, CHEN Yu-guo, PENG Ya-hui, ZHAO Hua, ZHANG Shu-gen

Chinese Journal of Energetic Materials, 2016, 24(7): 715–722

Executive editor: WANG Yan-xiu JIANG Mei ZHANG Qi