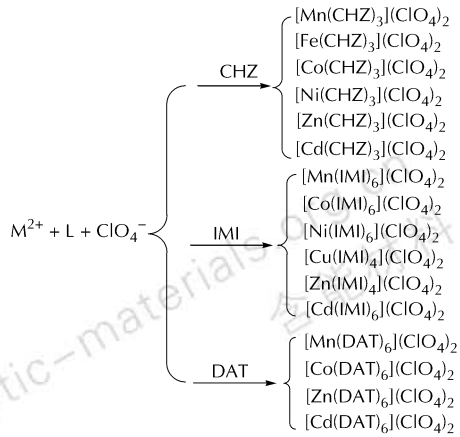
Recent Research Progresses in Energetic Coordination Compounds

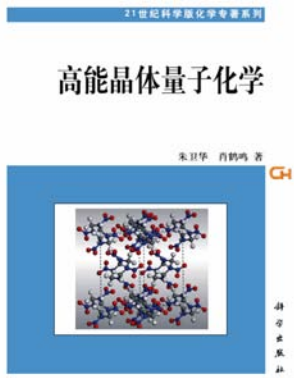


ZHANG Tong-lai, WU Bi-dong, YANG Li, ZHOU Zun-ning, ZHANG Jian-guo

Chinese Journal of Energetic Materials, 2013, 21(2): 137 −151

$[Zn(CHZ)_3](ClO_4)_2$ (GTX) and $[Cd(CHZ)_3](ClO_4)_2$ (GTG) are two important primary explosives with good thermal stability and sensitivity and applied industrially.

"Quantum Explosive Chemistry" and its Continuation—— Comment on "Prefaces" and "Forewords" of Several Academic Works



XIAO He-ming, ZHU Wei-hua, XIAO Ji-Jun, WANG Gui-xiang, LIU Dong-mei

Chinese Journal of Energetic Materials, 2013, 21(2): 152 −156

It is a cover of newly published book "Quantum Chemistry of Energetic Crystals", in which displays the unit cell of commonly used explosive HMX (1,3,5,7-tetranitro-1,3,5,7-tetrazocane).

Review on Carriers for Melt-cast Explosives

CAO Duan-lin, LI Ya-jin, DU Yao, WANG Jian-long, LI Yong-xiang

Chinese Journal of Energetic Materials, 2013, 21(2): 157 −165

The current research situation at home and abroad of four types of explosives which can be used as carriers for melt-cast explosive were summarized.

Some Problems in Theoretical Design of Energetic Materials

SHU Yuan-jie, LI Hua-rong, XIONG Ying, ZHOU Yang, QIAN Wen

Chinese Journal of Energetic Materials, 2013, 21(2): 166 −172

Some important problems in theoretical design of energetic materials were introduced, including the methods to evaluate the densities, heats of formation (HOFs), thermal decomposition mechanisms and detonation properties of usual energetic compounds, and moreover, to reveal the interface properties of energetic copolymers. The calculation of the above properties may provide useful information for the molecular design of novel high energetic density materials.

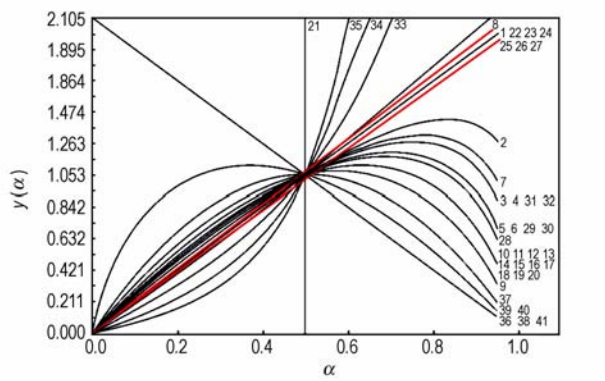
Progress in Oxidation-Coupling Reaction of Nitrogen-Containing Heterocyclic Compounds

XIAO Xiao, GE Zhong-xue, LIU Qing, XU Cheng, WANG Wei, SU Hai-peng , BI Fu-qiang

Chinese Journal of Energetic Materials,2013,21(2): 173 -179

Advances in oxidation-coupling reaction of hydrazo-azo and amino-azo in nitrogen-containing heterocyclic compounds were reviewed. The effects of different oxidants on oxidation-coupling reaction were discussed and the trends in the development of oxidation-coupling reaction of nitrogen-containing heterocyclic compounds were pointed out.

A Method of Computing/Determining the Arrhenius/non-Arrhenius Kinetic Parameters of the Exothermic Decomposition Reaction of Energetic Materials from Data of DSC Curves at Different Heating Rate



HU Rong-zu, MA Hai-xia, YAN Biao, ZHANG Hai, HAN Lu, GAO Hong-xu, ZHAO Feng-qi, YAO Er-gang, ZHAO Hong-an

Chinese Journal of Energetic Materials,2013,21(2): 180 -193

A method of computing/determining the Arrhenius/non-Arrhenius kinetic parameters of the exothermic decomposition reaction of energetic materials (EMs) was presented from initial temperature (T_e), peak temperature (T_p), conversion degree ($\alpha_{ei\ or\ pi}$) at $T_{ei\ or\ pi}$ and data (β_i, $T_{\alpha,i}$, $i=1,2,\cdots,L$) corresponding to isoconversation degree (α_i) for DSC curves under different constant heating rate (β) conditions.

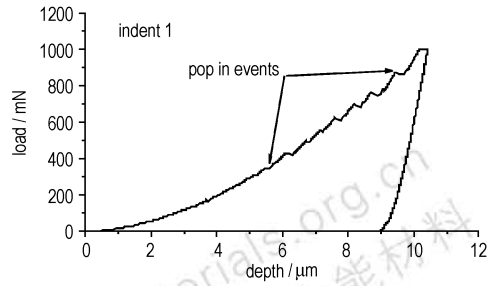
Designs and Synthetic Routes of Nitramine Explosives Containing Pyridine/Aminobenzene Ring

LU Ming, ZHAO Guo-zheng, NIE Fu-de, LI Jin-shan

Chinese Journal of Energetic Materials,2013,21(2): 194 -199

The insensitive property of explosives containing pyridine/aminobenzene rings is combined with the high energy of nitramine explosives, and the concept of new nitramine explosive containing pyridine/aminobenzene ring is proposed, into which the nitramine group with N—N bonds is introduced as much as possible. Based on the research of regular relationship between molecular as well as crystal structure and explosive property as well as security performance, the molecular structures of several target compounds and the synthetic method are designed. The synthetic routes are obtained with different synthetic reactions such as condensation, *N*-nitration, *N*-oxidation and *C*-nitration and so on.

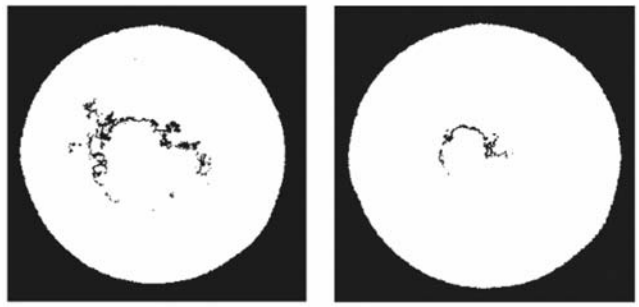
Ruptures and Mesoscale Fracture Behaviors of RDX Crystals



The regular "pop in" occurs on the loading/unloading curve, which shows mseoscal fracture takes place on face (210) of RDX crystal after initial elastic deformation.

LI Ming, CHEN Tian-nan, PANG Hai-yan, HUANG Ming
Chinese Journal of Energetic Materials,2013,21(2): 200 -204

Healing of Cracks in PBX by Thermal Pressure Aging Treatment



Thermal-pressure aging treatment was used in the study on cracks healing behavior of PBX. The cracks blow 400 μm healed after treated, and the internal quality of the damaged samples effectively was improved.

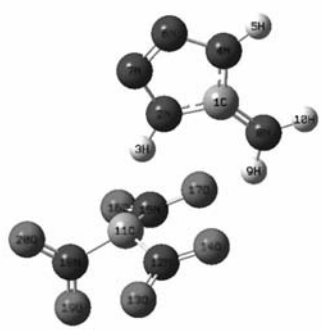
LAN Qiong, DAI Bin, YANG Bai-feng , LI Jing-ming, HE Jian-hua
Chinese Journal of Energetic Materials,2013,21(2): 205 -208

Application of PDADN in Screw Extruded Nitramine Modified Double-base Propellant

several screw extruded nitramine modified double-base propellant were experimentally analyzed. Effects of the pentaerythrite diazidodinitrate (PDADN) on the mechanical property, burning characteristic, chemical stability, mechanical sensitivity, energy characteristic and gas characteristic signal of propellant were studied.

LIU Suo-en, ZHOU Wei-liang, PAN Bao, ZHAO Mei-ling, ZOU Wei-wei
Chinese Journal of Energetic Materials,2013,21(2): 209 -212

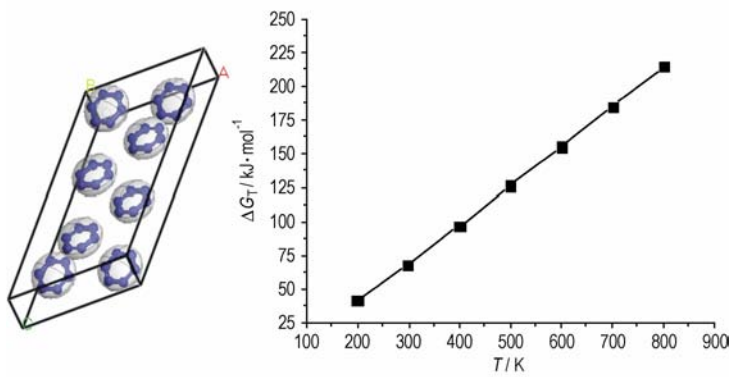
Theoretical Computation of 5-Aminotetrazolium Nitroformate



The structure of 5-aminotetrazolate nitroformate was optimized by a B3LYP method based on 6-31G(d) basis set using Gaussian 03 program. The density, heat of formation, detonation velocity and detonation pressure were calculated.

LIU Wei, LI Yu-chuan, LI Xiao-tong, YANG Yu-zhang, LIN Qiu-han, PANG Si-ping
Chinese Journal of Energetic Materials,2013,21(2): 213 -216

Structure and Synthetic Feasibility of Pseudo-benzene N_6

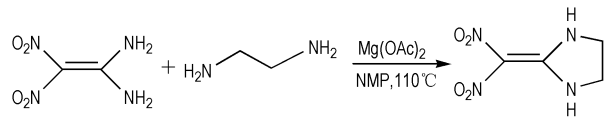


Fully optimized calculation and vibrational analysis for nitrogen and pseudo-benzene N_6 were carried out using density-functional theory (DFT) method at B3LYP/6-311 + + G(d, p) level. Molecular mechanics (MM) method with Compass and Dreiding force fields was used to predict molecular packing for N_6 among the 7 most probable space groups ($P2_1/c$, P-1, $P2_12_12_1$, $P2_1$, $Pbca$, $C2/c$, and $Pna2_1$), respectively. The feasibility of process was analyzed with thermodynamics and reaction mechanism was predicted.

ZHAO Guo-zheng, LU Ming

Chinese Journal of Energetic Materials, 2013, 21(2): 217 -221

Synthesis of 2-(Dinitromethylene)-1, 3-diazacyclopentane (DNDZ) Catalyzed by Magnesium Ion

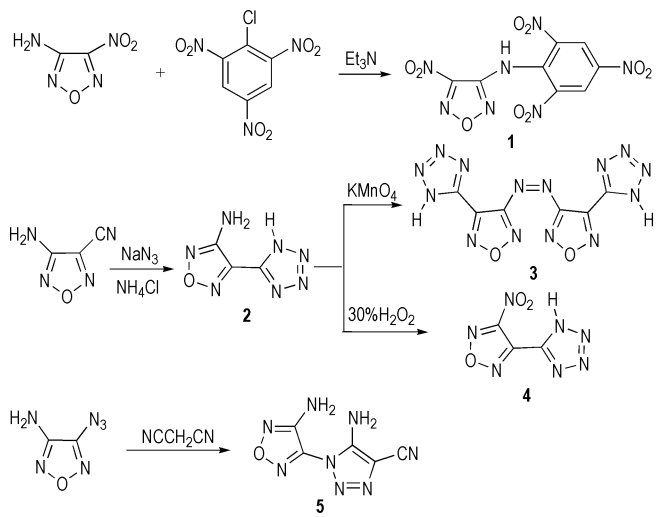


As an important intermediate for new energetic materials, 2-(dinitromethylene)-1, 3-diaza- cyclopentane(DNDZ) prepared by the necleophilic reaction between 1,1-diamino-2,2-dinitroethylene(FOX-7) and 1,2-diaminoethane catalyzed by magnesium ion had been studied and the DNDZ was synthesized in yield of 83.9% with high purity (99%) under the optimum conditions: new $Mg(OAc)_2$ as the catalyst and the content was 30%.

LIU Pan, XU Zhi-bin, WANG Bo-zhou, GE Zhong-xue, WANG Peng, MENG Zi-hui

Chinese Journal of Energetic Materials, 2013, 21(2): 222 -225

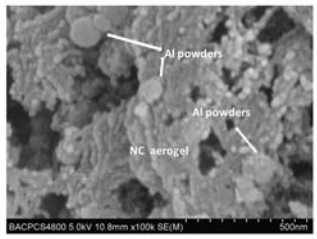
New Synthetic Route of Five Furazan Derivatives



GAO Li, YANG Hong-wei, WU Bo, CHENG Guang-bin, Lü Chun-xu

Chinese Journal of Energetic Materials, 2013, 21(2): 226 -229

Preparation and Characterization of NC/Al Nano-composite Energetic Materials

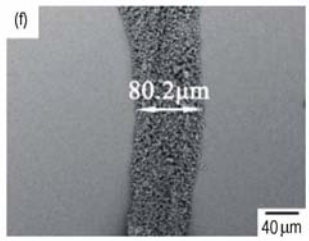


JIN Miao-miao, LUO Yun-jun

Chinese Journal of Energetic Materials,2013,21(2): 230 -234

The NC/Al nano-composite materials were prepared through sol-gel and supercritical carbon dioxide drying methods. The nano-composite material was characterized by FTIR, BET, SEM and DSC methods, and the results show that the nano-composite material process different thermal properties from the NC-gel/Al physical mixture and NC/Al physical mixture.

Preparation and Characterization of Direct Write Explosive Ink Based on CL-20

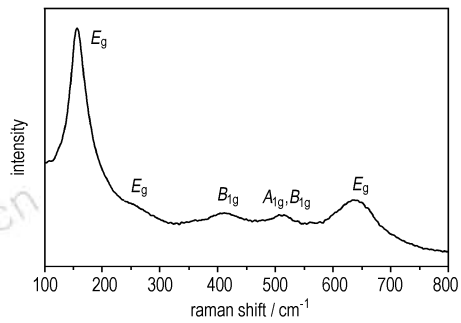


ZHU Zi-qiang, CHEN Jin, QIAO Zhi-qiang, HUANG Bing, YANG Guang-cheng, NIE Fu-de

Chinese Journal of Energetic Materials,2013,21(2): 235 -238

A direct write explosive ink CL-20 based was prepared. Its direct write property and detonation performance were studied by SEM, FTIR and wedge shaped charge test, respectively.

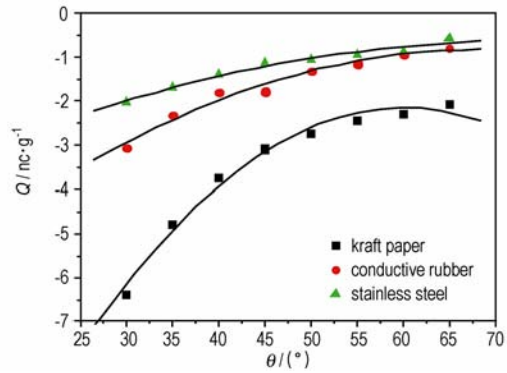
Preparation of AC/TiO_2 Composite Particles at Low Temperature and its Application in Degradation of TNT Wastewater



DU Shi-guo, YAN Jun, WANG Ming-qiu, WANG Bin

Chinese Journal of Energetic Materials,2013,21(2): 239 -243

Electrostatic Accumulation Test of Initiating Explosives

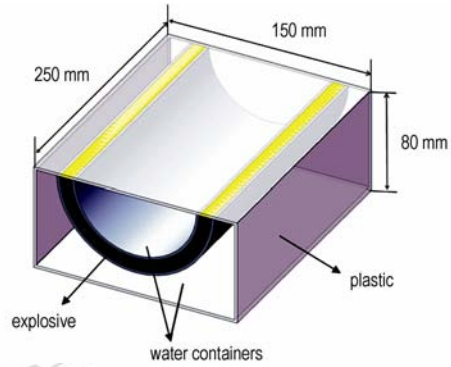


ZHOU Ming-rui, LI Zhi-min, ZHANG Tong-lai, WU Bi-dong, YANG Li, ZHANG Jian-guo, ZHOU Zun-ning

Chinese Journal of Energetic Materials,2013,21(2): 244 -248

With quartz sands as the standard sample, the influences of testing conditions on the quartz sand electrostatic accumulation were analyed.

Numerical Study on Water Jet Formation of Semi-ring Shaped Charge

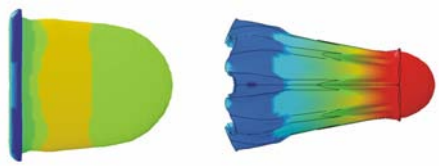


PEI Hong-bo, JIAO Qing-jie, NIE Jian-xin

Chinese Journal of Energetic Materials,2013,21(2): 249 -252

A device for disruption of explosive was proposed. Finite element program AUTODYN was used to simulation the forming progress of water jet.

Numerical Simulation of a Dual-mode EFP Warhead

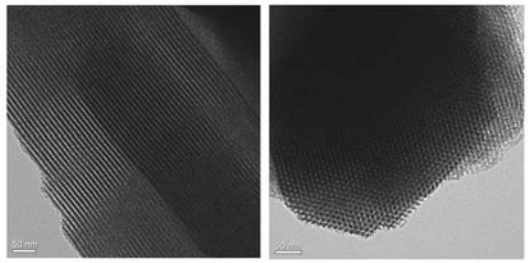


ZANG Li-wei,YIN Jian-ping,WANG Zhi-jun

Chinese Journal of Energetic Materials,2013,21(2): 253 -256

The liner which fixed grooved torus could form EFP with fin, the length-diameter ratio of EFP with fins is 2.75 times of that of EFP and its velocity increased 15 percent.

Ammonium Perchlorate Oxidation for Removal of Organic Templates to form SBA-15 Type Material

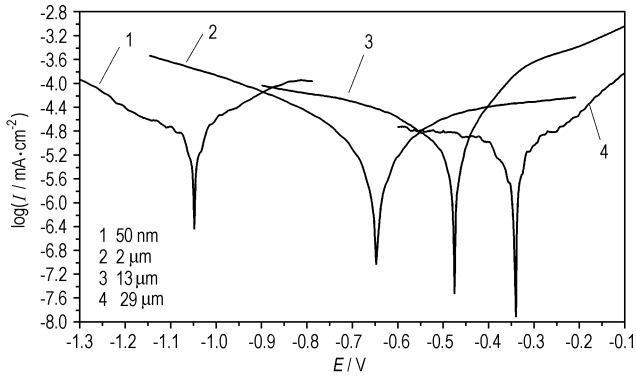


YANG Rong-ji, CAI Hua-qiang, TIAN Li, JIANG Kai, HUANG Hui

Chinese Journal of Energetic Materials,2013,21(2): 257 -261

Organic templates were removed by AP-HNO_3 oxidation at 100 ℃ to form high quality mesoporous silica N-SBA-15.

Reaction of Al Powder and Water Visa Electrochemistry Technology

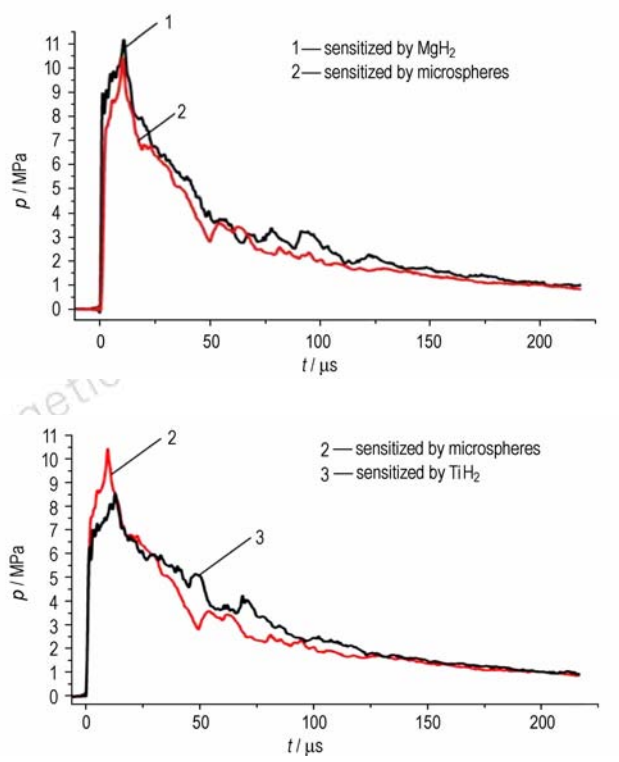


TONG Da-ming, CAI Shui-zhou, XIE Chang-sheng, XIA Xian-ping, ZENG Da-wen

Chinese Journal of Energetic Materials,2013,21(2): 262 -267

Al powder with 50 nm, 2 μm,13 μm and 29 μm was studied from the perspective of electrochemistry. The behaviours of Al-H_2O reaction affected by particle size and temperature were discussed. The electrochemical thermodynamic parameters of Al-H_2O reaction were calculated.

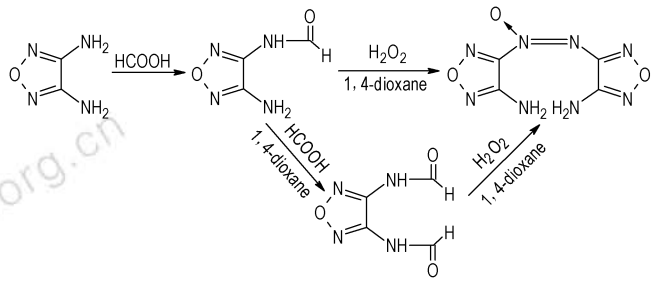
Hydrogen Storage Materials Applied in Emulsion Explosives



CHENG Yang-fan, LIU Rong, MA Hong-hao, SHEN Zhao-wu
Chinese Journal of Energetic Materials,2013,21(2): 268 -272

Hydrogen storage material MgH_2 and TiH_2 played double roles in the explosives which acted as sensitizers and energetic materials and significantly improved emulsion explosives energy output characteristic.

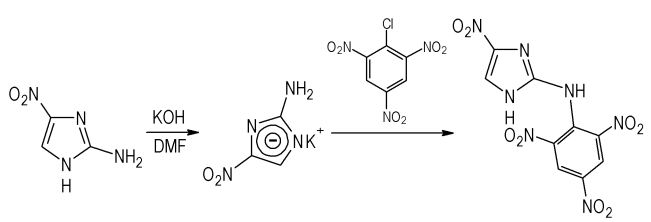
A New Method to Synthesize 3,3′-Diamino-4,4′-azoxyfurazan (DAOAF)



DAOAF was synthesized from 3,4-diaminofurazan, which used 3-amino-4-formylaminofurazan or 3,4-diformylaminofurazan as intermediate, 1,4-dioxane as solvent, and 30% H_2O_2 as a oxidant by refluxing for 4 h, and yield 97% or 89%.

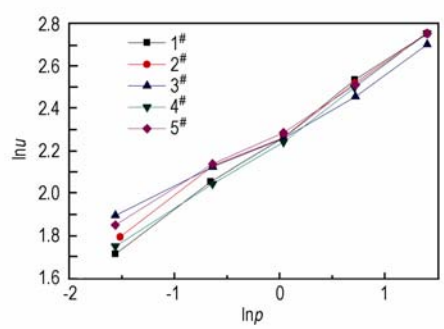
WU Min-jie, CHEN Shu-sen, JIN Shao-hua, LI Li-jie
Chinese Journal of Energetic Materials,2013,21(2): 273 -275

Synthesis and Thermal Behavior of 2-(2,4,6-Trinitro)phenylamino-4-nitroimidazole



JIA Kai, LIU Zu-liang, HOU Ke-hui
Chinese Journal of Energetic Materials,2013,21(2): 276 -277

RDX/HMX Effects on Combustion Performance of Boron-based Fuel-rich Propellant

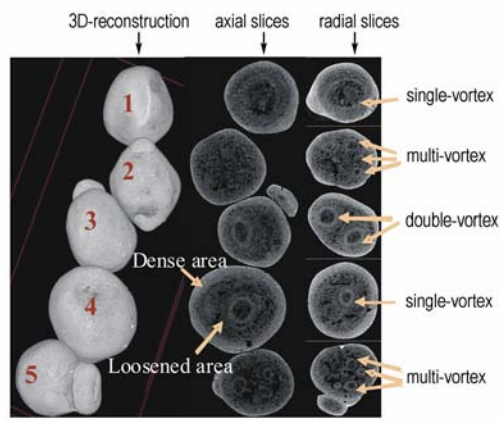


Five boron-based fuel-rich propellants containing RDX/HMX were prepared to explore the effect of RDX/HMX on the combustion performance of the boron fuel-rich propellant by the measurement of burning rate, explosion heat, combustion temperature and combustion gas generation rate of the propellants.

LIU Lin-lin, HE Guo-qiang, WANG Ying-hong

Chinese Journal of Energetic Materials, **2013**, **21**(**2**): **278**

Microstructures Characterization of TATB Based Granules by High Resolution X-ray Computed Tomography



HRXCT scans of the TATB based granules show that they are fully like vortex-cores & dense-crusts structure. The condensed vortex rings are preserved by condensation and encrustation with binder, and differences in X-ray attenuation provide more details about their distribution.

ZHANG Wei-bin, DAI Bin, YANG Xue-hai, TIAN Yong, XIAO Li, YANG Cun-feng, YANG Reng-cai

Chinese Journal of Energetic Materials, **2013**, **21**(**2**): **279 -280**

Executive editor: WANG Yan-xiu JIANG Mei; Computer typesetter: ZHANG Gui-hong