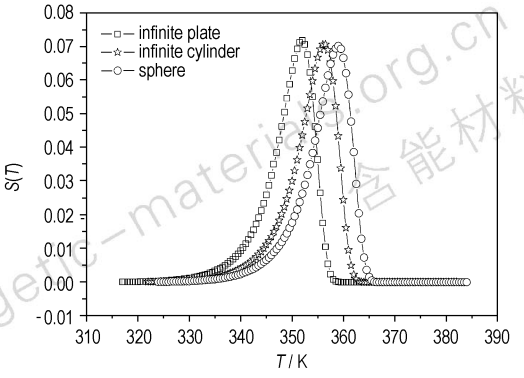
The Thermal Safety and a Density Functional Theoretical Study on *N*, *N*′-Bis[*N*-(2,2,2-Trinitroethyl)-*N*-Nitro] Ethylenediamine (BTNEDA)

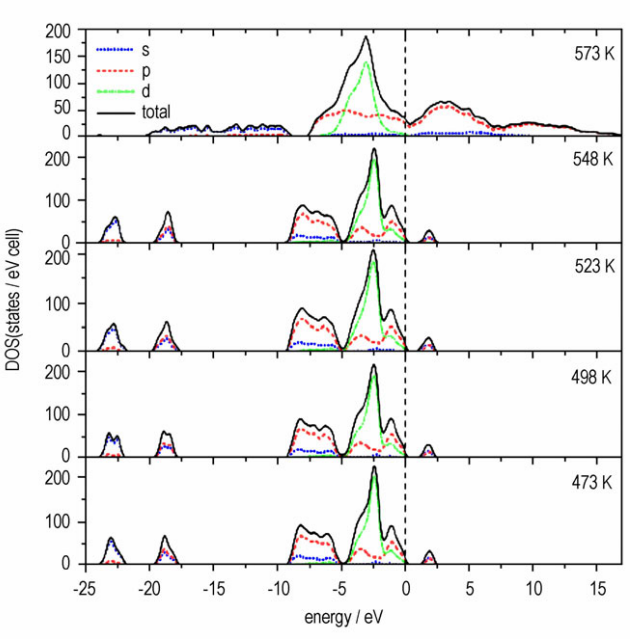


HU Rong-zu, ZHAO Feng-qi, GAO Hong-xu, MA Hai-xia, ZHANG Hai, XU Kang-zhen, ZHAO Hong-an, YAO Er-gang

Chinese Journal of Energetic Materials, 2012, 20(5): 505 −513

The values of specific heat capacity, thermal conductivity, standard combustion energy and standard enthalpy of formation of BTNEDA were estimated. The validity of the values of apparent activation energy obtained by non-isothermic method was checked by an isothermal method. Adiabatic time-to-explosion, 50% drop height of impact sensitivity, critical temperature of hot-spot initiation, thermal sensitivity probability density function, safety degree, critical thermal explosion ambient temperature and thermal explosion probability of BTNEDA were calculated. Information was obtained on thermal safety of BTNEDA. The conjunction of BTNEDA was optimized with density functional theory (DFT) B3LYP. The atomic charges, total energy and frontier orbital energy were also discussed.

Theoretical Studies on Sensitivity Criterion of Energetic Materials——From molecules, crystals, to composite materials

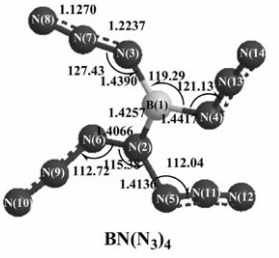


XIAO He-ming, ZHU Wei-hua, XIAO Ji-Jun, WANG Gui-xiang, PEI Xiao-qin

Chinese Journal of Energetic Materials, 2012, 20(5): 514 −527

We review the thermal decomposition mechanisms and sensitivity criterions of energetic molecules, crystals, and composite materials based on our theoretical studies.

Molecular Design and Theoretical Study on Novel High-nitrogen Energetic Azido Compounds

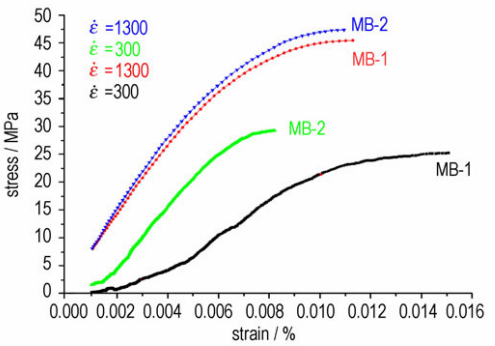


$BN(N_3)_4$

MAN Tian-tian, NIU Xiao-qing, ZHANG Jian-guo, WANG Ying, ZHANG Tong-lai, ZHOU Zun-ning
Chinese Journal of Energetic Materials, **2012**, **20**(**5**): **528 −533**

Seven high-nitrogen energetic compounds were devised: $C(N_3)_4$, $B(N_3)_3$, $N(N_3)_3$; $CC(N_3)_4$, $BN(N_3)_4$, $NN(N_3)_4$ and $CC(N_3)_6$, which are structurally similar to CH_4, BH_3, NH_3 and C_2H_4. The molecular geometries, IR spectra, bond order and frontier orbital energies of these compounds were obtained at B3PW91/6-311+G(d) level of theory.

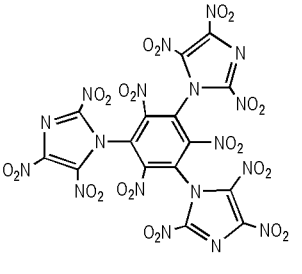
Performance of Modified Composition B with Thermoplastic Elastomer



GAO Da-yuan, WEN Wen, SHU Yuan-jie, HUANG Qian, CAI Zhong-zhan, WEN Mao-ping, LAN Lin-gang, LUO Guan
Chinese Journal of Energetic Materials, **2012**, **20**(**5**): **534 −540**

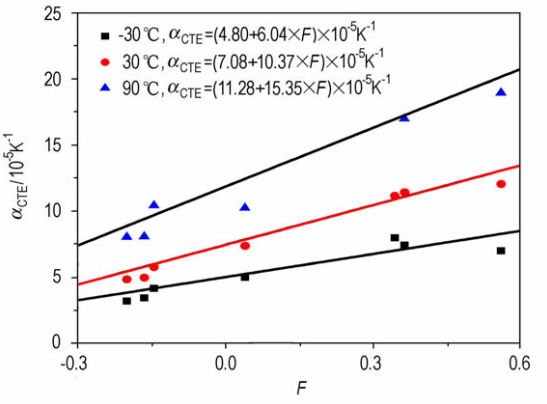
The elasticity and toughness of the MB-1 and MB-2 were better than that of Comp. B. The toughness of MB-2 was better than that of MB-1 in low speed impact experiment. The impact sensitivity of the MB-1 was higher than that of MB-2. Compared with Comp. B, the CJ velocities and CJ pressures of MB-1 and MB-2 decrease slightly.

Empirical Calculation of the Explosion Parameters of Nitrodiazole Explosives



WANG Jun, DONG Hai-shan, LI Jin-shan, SHU Yuan-jie
Chinese Journal of Energetic Materials, **2012**, **20**(**5**): **541 −544**

Influence of Crystal Preferred Orientation on Thermal Expansion of Die Pressed TATB Based PBXs

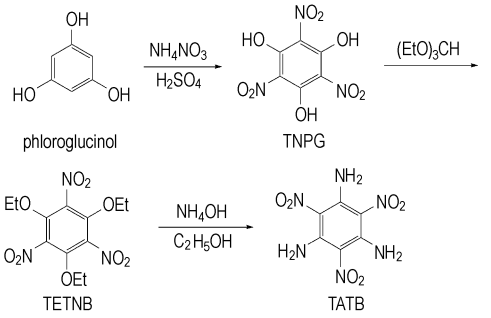


SUN Jie, ZHANG Hao-bin, WEN Mao-ping, ZHANG Qiu, LIU Xiao-feng

Chinese Journal of Energetic Materials,2012,20(5): 545 -550

It's shown that die-pressed TATB cylinders usually take place anisotropic thermal expansion with the coefficient of thermal expansion (CTE) along the diameter and that along the radial satisfy the formula $\alpha_{CTE} = (7.08 + 10.37 \times F) \times 10^{-5} K^{-1}$. We can try to control the preferred orientation by change the crystal morphology, further to restrain the anisotropy of thermal expansion, and finally to improve the shape stability of TATB cylinders.

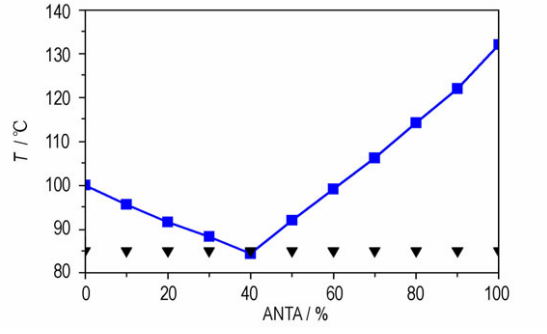
Improvement of Synthesis Technology of TATB Free from Chloride



HUANG Jing-lun, ZHANG Li-yuan, MA Qing, WANG Zheng

Chinese Journal of Energetic Materials,2012,20(5): 551 -554

Preparation and Properties of Lowest Eutectic Mixture TNAZ/ ANTA

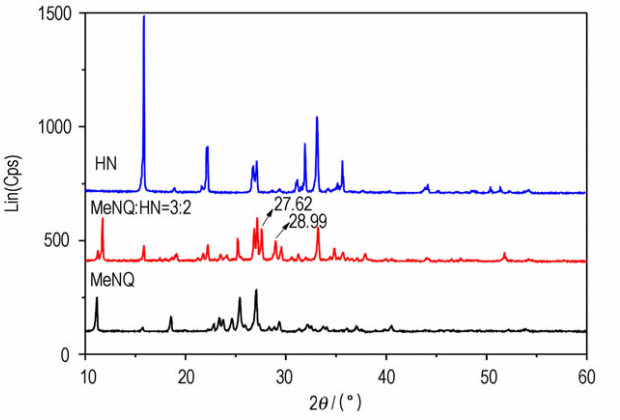


ZHANG Xue-mei, DONG Hai-shan, SUN Jie, GAO Da-yuan, XIA Yun-xia, LIU Xiao-feng, DONG Xiao

Chinese Journal of Energetic Materials,2012,20(5): 555 -559

A phase diagram of 1,3,3-trinitroazetidine(TNAZ) and 3-amino-2,4,6-trinitroanisole (ANTA) was obtained. The sensitivity, thermal stability, and detonation performance of the eutectic mixture were tested and the results showed that the eutectic mixture was a potential replacement of TNT for melt-cast explosive.

Structure and Molecular Interaction of Methyl-nitroguanidine and Hydrazine Nitrate Eutectics

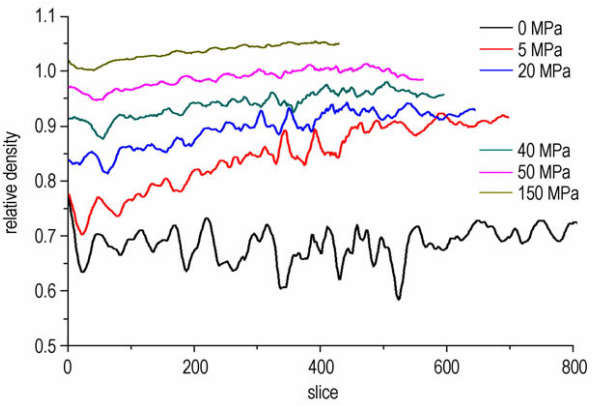


CHEN Ling, LI Hua-rong, XIONG Ying, XU Rui-juan, XU Tao, LIU Xiao-feng, SHU Yuan-jie

Chinese Journal of Energetic Materials,2012,20(5):560 -564

The melt point, crystal shape, structures and interaction of different mole contents of methyl-nitroguanidine and hydrazine nitrate were tested by differential scanning calorimeter(DSC), optical microscope, X-ray diffraction(XRD) and density functional theory respectively.

Density Distribution of Pressed RDX Crystals with a Cone-beam Micro-focus Computed Tomography

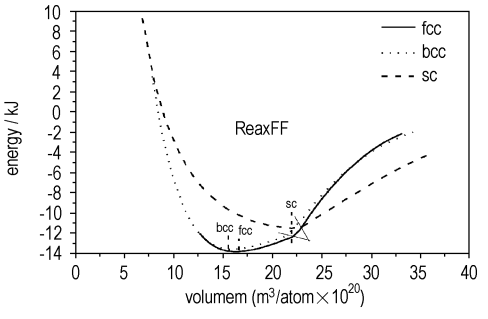


ZHANG Wei-bin, TIAN Yong, YANG Reng-cai, DAI Bin, YANG Xue-hai

Chinese Journal of Energetic Materials,2012,20(5):565 -570

All section density of explosive grow up with the increase of pressure, the closer to the press end, the more the density increases, the fluctuation and gradient of the density gradually reduce as the pressure increases.

Applicability of ReaxFF Potential in Aluminum

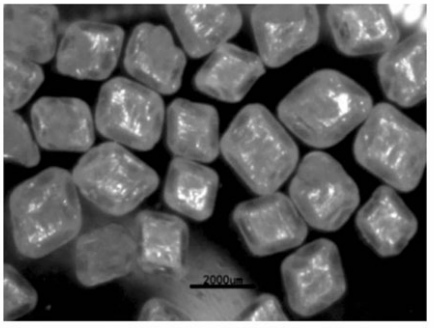


SONG Wen-xiong, ZHAO Shi-jin

Chinese Journal of Energetic Materials,2012,20(5):571 -574

In order to evaluate the applicability of ReaxFF in Aluminum, some physical properties about aluminum were calculated by reaction force field (ReaxFF), and compared with embedded atom method (EAM), DFT and the experimental value.

Experimental Research and Mechanism on Re-crystallization of HMX in PC Solvent

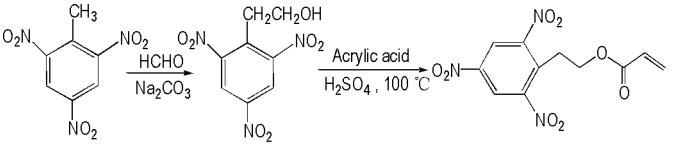


Results indicate that adding crystal seeds could inhibit generation of HMX twin-crystals in crystallization process and extending crystallization time is conribute larger to crystals formation.

GAO Feng, HUANG Hui, HUANG Ming, DUAN Xiao-hui

Chinese Journal of Energetic Materials,2012,20(5): 575 -578

Synthesis and Thermal Decomposition Performance of Acrylic 2,4,6-Trinitrophenethyl Ester

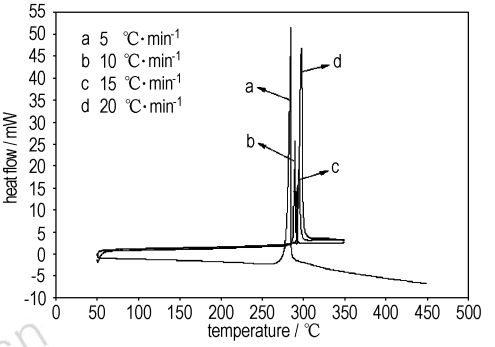


A new energetic material acrylic 2,4,6-trinitrophenethyl ester was synthesized through the reactions of 2,4,6-trinitrotoluene (TNT), formaldehyde and acrylic acid.

LIU Qiang-qiang, JIN Bo, PENG Ru-fang, SHU Yuan-jie, CHU Shi-jin, DONG Hai-shan

Chinese Journal of Energetic Materials,2012,20(5): 579 -582

Thermal Behavior of 3-Nitro-5-guanidino-1,2,4-oxadiazole

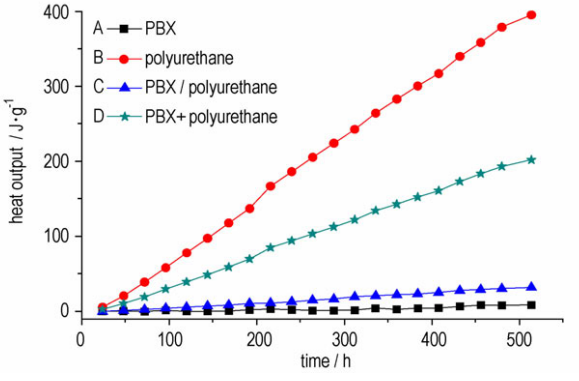


The thermal behavior and non-isothermal decomposition kinetics of 3-nitro-5-guanidino-1,2,4-oxadiazole (NOG) were studied by DSC and TG-DTA.

FU Zhan-da, WANG Yang, CHEN Fu-xue

Chinese Journal of Energetic Materials,2012,20(5): 583 -586

Compatibility of HMX Based PBX Specimens and Polyurethane Gum

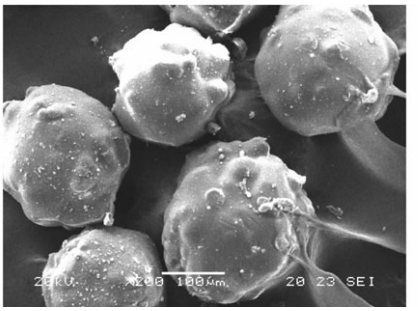


The reactivity and compatibility between HMX based PBX specimens and polyurethane gum were studied by microcalorimetry, TG-DSC and FTIR.

ZUO Yu-fen, XIONG ying, CHEN jie, XIA Jing-qiong, WANG lin

Chinese Journal of Energetic Materials,2012,20(5): 587 -591

Effects Composite Spherical Propellants on Improvement of Mechanical and Combustion Properties of Modified Double-based Propellant

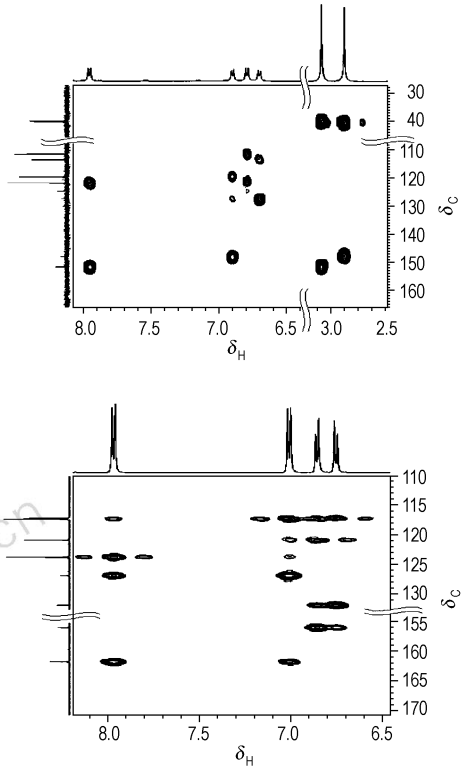


Al powder, RDX and catalysts was coated by nitrocellulose and formed composite spherical green powder. Results indicate composite spherical green powder is contribute to improvement interface bonding between fillers and adhesive matrix.

ZHU Lin, OU Jiang-yang, YANG Xiao-yu, WANG Yan-jun

Chinese Journal of Energetic Materials, **2012**, **20**(**5**): **592** −**595**

Synthesis and NMR Characterization of *p*-Dimethylaminophenylpentazole and *p*-Hydroxyphenylpentazole at Low Temperature

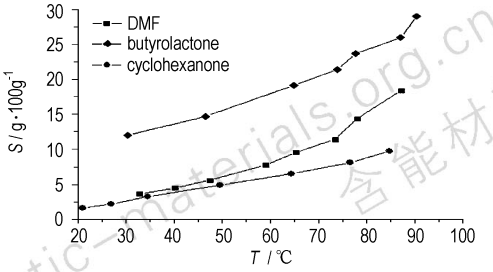


p-Dimethylaminophenylpentazole (*p*-DMAPP) and *p*-hydroxyphenylpentazole (*p*-HPP) were synthesized at −40 ℃, using *N*1, *N*1-dimethylbenzene-1,4-diamine and 4-aminophenol as starting meaterials, respectively. Their stuctures were characterized by ^{1}H NMR, ^{13}C NMR, ^{1}H-^{13}C HMBC, ^{15}N NMR and ^{1}H-^{15}N HMBC at low temperature.

XU Min, BI Fu-qiang, ZHANG Gao, WANG Min-chang, GE Zhong-xue, CHEN Zhi-qun, XU Cheng

Chinese Journal of Energetic Materials, **2012**, **20**(**5**): **596** −**600**

Determination and Correlation of HMX Solubility by FBRM

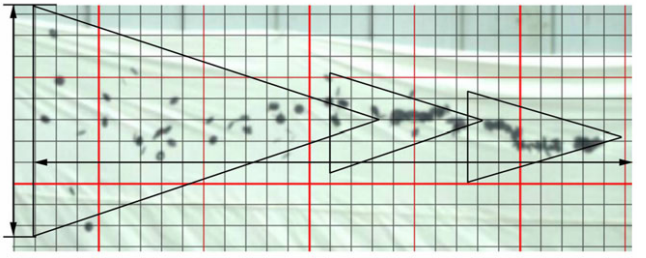


The dynamic online analysis system composed of focused beam reflectance measurement (FBRM) and automated lab reactor (Labmax) was used to determine the solubility of HMX in *N*,*N*-dimethylformamide (DMF), 1,4-butrolactone and cyclohexanone. The measured solubility was correlated with Apelblat model and polynomial empirical equation, respectively.

LIN He, ZHU Shun-guan, LI Hong-zhen, ZHANG Lin, HU Jian-ju

***Chinese Journal of Energetic Materials*,2012,20(5): 601 −604**

Dispersing Experiment for Separation and Dispersion of Multi-plates

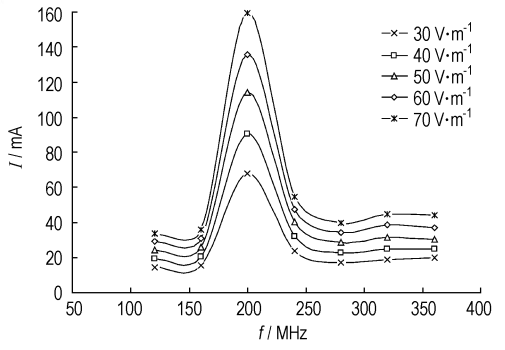


A mass of plates disperse when a dispersing experiment was carried out. The plates separate from the tail of cluster due to the aerodynamic. The cluster separates into several parts and disperses scheduling. Each part shows a cone shape.

HUANG Bei, WANG Hao, WANG Shuai, GUO Jin-yan

***Chinese Journal of Energetic Materials*,2012,20(5): 605 −609**

Response Rule of Hot-wire EED in Continuous Electromagnetic Environment

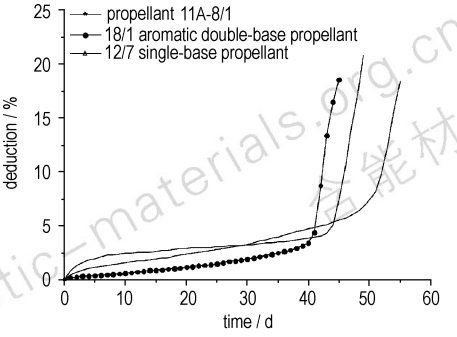


In order to explore the hot-wire EED′s response rules in continuant electromagnetic environment, utilizing an electromagnetic radiation experiment system, the influence of important parameters were studied.

WANG Ke-xuan, BAI Ying-wei, REN Wei, CHENG Jia-qi

***Chinese Journal of Energetic Materials*,2012,20(5): 610 −613**

Chemical Stability of Di-stabilizers Propellants and Corresponding Reaction Mechanism



NIU Jia-xin, SUN Gui-zhi, ZHANG Yu-qing, WANG Bo, LI Yong, SUN Hai-quan

Chinese Journal of Energetic Materials, **2012**, **20**(**5**): **614 −617**

The chemical stability of di-stabilizers single-based propellant with diphenylamine(DPA) and centralite Ⅱ used as stabilizer heated at 75 ℃, 85 ℃, 90 ℃ and 95 ℃ was studied by a multi-temperature artificial accelerated ageing test, and gas-chromatography (GC), respectively.

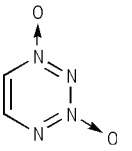
Toughening and Elasticizing Route of TNT Based Melt Cast Explosives

MA Qing, SHU Yuan-jie, LUO Guan, CHEN Ling, ZHENG Bao-hui, LI Hua-rong

Chinese Journal of Energetic Materials, **2012**, **20**(**5**): **618 −629**

Brittleness and cracks in melt cast explosives restrain the application in high performance weapon systems. A systematic overview of TNT based melt cast explosives in toughening and elasticizing experiments is given. New toughening and elasticizing techniques, and computational research on interaction of components in melt cast explosives are introduced.

Progress in the Energetic Materials Based on 1,2,3,4-Tetrazine 1,3-Dioxide



BI Fu-qiang, WANG Bo-zhou, LI Xiang-zhi, FAN Xue-zhong, XU Cheng, GE Zhong-xue

Chinese Journal of Energetic Materials, **2012**, **20**(**5**): **630 −637**

1,2,3,4-Tetrazine 1,3-dioxide is a potential energetic moiety in the design and synthesis of high energy density materials. The synthetic methods of 1,2,3,4-tetrazine 1,3-dioxide were summarized and the research progresses in benzo(pyrido)-1,2,3,4-tetrazine 1,3-dioxide and its derivatives, nonannulated 1,2,3,4-tetrazine 1,3-dioxides, furazano[3,4-e]-1,2,3,4-tetrazine 4,6-dioxide (FTDO) and 1,2,3,4-tetrazino[5,6-e]-1,2,3,4-tetrazine 1,3,5,7-tetraoxide (TTTO) were reviewed with **34** references quoted.

Development of Isostatic Pressing Technology of Explosive Charge

SUN Jian

Chinese Journal of Energetic Materials, **2012**, **20**(**5**): **638 −642**

The technological characteristics and method of molding of the explosive by isostatic pressing were outlined. The current research situation of the isostatic pressing technology of explosive charge was summarized. Suggestions on the application of isostatic pressing technology of explosive charge from highend to conventional were presented for the conventional warhead development requirements of the high quality technology of explosive charge.

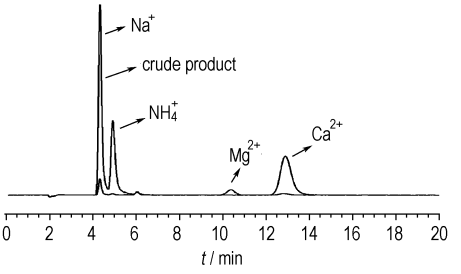
Review on Realationships Between the Molecular and Crystal Structure of Explosives and Their Sensitivities

CAO Xia, XIANG Bin, ZHANG Chao-yang

Chinese Journal of Energetic Materials,2012,20(5): 643 -649

The sensitivities of explosives are governed by their multiscale structures, among which the explosive molecules and crystals are the bases of these structures and the factors determining their structures and the properties in principle. It is a hotspot to study the relationship between the sensitivity and the molecular and crystal stucture of explosive in energetic material (EM).

Determination of Ionic Residues in 3,4-Dinitrofurazan by Ionic Chromatography

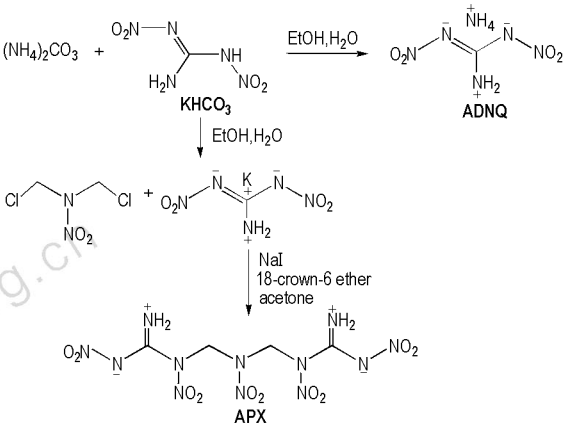


XUE Min, ZHONG Xu, MENG Zi-hui, CHEN Zhi-qun, XU Min, JIA Lin, ZHANG Gao

Chinese Journal of Energetic Materials,2012,20(5): 650 -652

Concentrations of trace anions and cations as Na^+, Mg^{2+}, Ca^{2+}, $HCOO^-$, Cl^-, NO_2^-, and NO_3^- presented in with and without refined 3,4-dinitrofurazan products were determined by ion chromatography method considering their influences on the explosive manufacturing process.

Synthesis of Two Novel Explosives Based on 1,2-Dinitroguanidine



YANG Wei, WANG Bo-zhou, WANG You-bing, LI Ya-nan

Chinese Journal of Energetic Materials,2012,20(5): 653 -655

Using 1,3-dichloro-2-nitrazapropane and potassium dinitroguanidine as starting materials, 1,7-diamino-1,7-dinitrimino-2,4,6-triazaheptane (APX) was synthesized by condensation with sodium iodide and 18-crown-6. Ammonium-dinitroguandine (ADNQ) was synthesized by 1,2- nitroguanidine and ammonium carbonate.

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