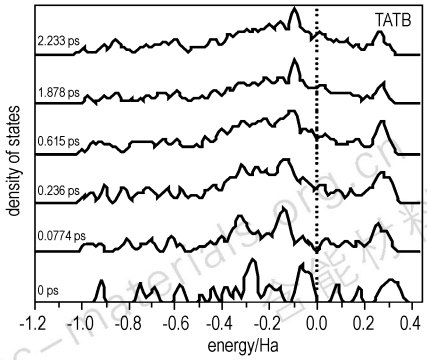
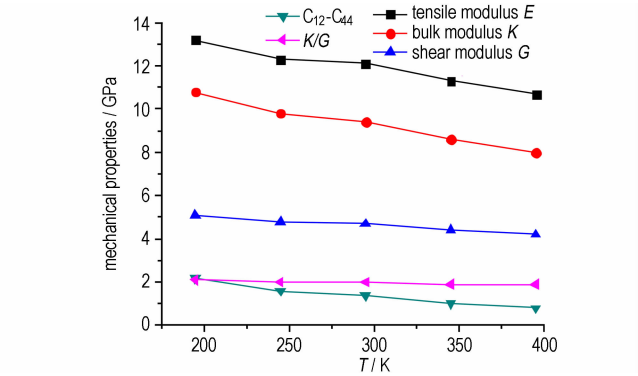
Initial Decomposition Mechanisms of Three Explosive Crystals under Shock Loading by Ab Initio Molecular Dynamics



Ab initio molecular dynamics in conjunction with multiscale shock technique was used to study the initial decomposition of HMX, TATB, and PETN crystals under shock wave loading.

ZHU Wei-hua, HUANG Hui, HUANG Heng-jian, XIAO He-ming
Chinese Journal of Energetic Materials,2013,21(5):557 −562

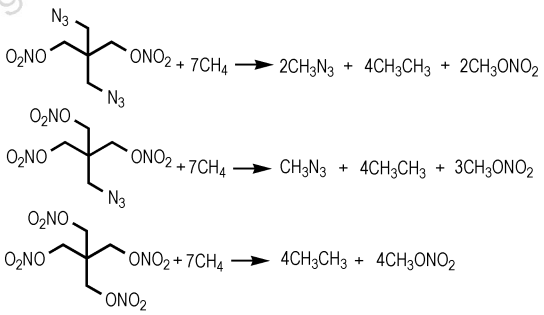
Sensitivity Criterion and Mechanical Performances Prediction of PETN Crystals at Different Temperatures by Molecular Dynamics Simulation



Two different PETN crystalline models were simulated at five different temperatures by molecular dynamics (MD) simulation using COMPASS force field in the isothermal-isobaric (NPT) ensemble. The trigger bond length, the interaction energy between two atoms of the trigger bond and the cohesive energy density as well as the mechanical properties of the PETN crystal were presented and analyzed.

LIU Dong-mei, XIAO Ji-jun, ZHU Wei, XIAO He-ming
Chinese Journal of Energetic Materials,2013,21(5):563 −569

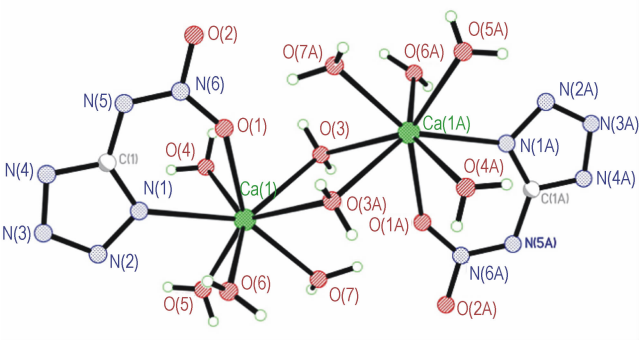
Theoretical Study on Detonation Properties and Pyrolysis Mechanism of Pentaerythritol Tetranitrate and its Analogue Compounds



A systematic theoretical study was carried out on tetraazido pentaerythritol (TAPE), pentaerythritol triazido nitrate (PTAN), pentaerythritol diazido dinitrate (PDADN), pentaerythritol azido trinitrate (PATN) and pentaerythritol tetranitrate (PETN) to investigate their structures and properties, especially the pyrolysis mechanism by analyzing the bond dissociation energy (E_{BD}) of the possible trigger bond and the activation energy (E_a) of the hydrogen transfer reaction.

YANG Jun-qing, WANG Gui-xiang, GAO Pin, GONG Xue-dong
Chinese Journal of Energetic Materials,2013,21(5):570 −577

Crystal Structure of a Novel Green Initiating Explosive Calcium Nitriminotetrazolate Pentahydrate

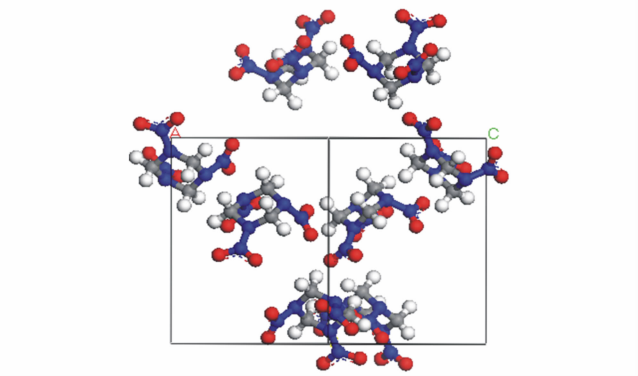


The structure of calcium nitriminotetrazolate pentahydrate [$Ca(NATZ)(H_2O)_5$] was determined by X-ray single crystal diffraction. Theoretical investigation was carried out by HF/6-311g and B3LYP/6-311g methods. This coordination compound has lower thermal stability.

TONG Wen-chao, WANG Shi-wei, WU Bi-dong, YANG Li, ZHANG Tong-lai

Chinese Journal of Energetic Materials **,2013,21(5): 578 –582**

Molecular Modeling and Prediction of RDX Crystal Morphology

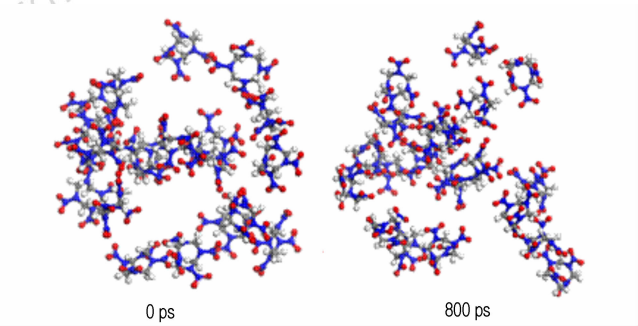


On the basis of the structure of α-RDX crystal, RDX crystal morphology was predicted by using the BFDH(Bravais-Friedel-Donnary-Harker) and AE(attachment energy) models. According to the surface structure, it can be to predict the effect of solvent on the crystal morphology.

CHEN Gang, WANG Feng-yun

Chinese Journal of Energetic Materials **,2013,21(5): 583 –588**

Molecular Dynamics Simulation of Crystallization of HMX Solution

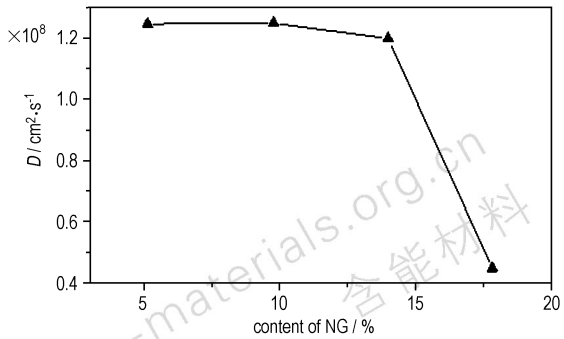


The effect of temperature on the crystallization of cyclotetramethylene tetranitramine (HMX) in dimethylsulfoxide (DMSO) solvent was investigated by molecular dynamics simulation. The diffusion coefficients of DMSO and HMX and binding energy between HMX and DMSO were calculated in 278 –378 K. The process of nucleus formation of HMX was simulated at 298 K.

YU Hai-li, DUAN Xiao-hui, TAN Xue-rong

Chinese Journal of Energetic Materials **,2013,21(5): 589 –593**

Molecular Dynamics Simulation of the Diffusion Behaviors of NG in Polyurethane

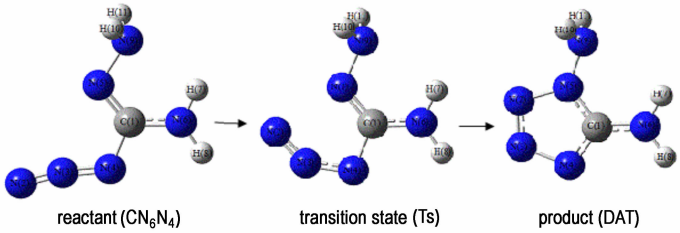


WANG Xiao, YAO Da-hu, BAI Sen-hu, WANG Cun-dong, HE Yu-xin, ZHANG Yu-qing

Chinese Journal of Energetic Materials, 2013, 21(5): 594 -598

The influences of temperature, content of nitroglycerin (NG), structure of diisocyanate on the diffusion behaviors of NG in elastomeric polyurethane were investigated by the molecular dynamics method with COMPASS force field.

Theoretical Studies on Kinetics of Isomerization Reaction for 1,5-Diamino-tetrazole



HE Piao, ZHANG Jian-guo, MAN Tian-tian, WANG Kun, ZHANG Shao-wen

Chinese Journal of Energetic Materials, 2013, 21(5): 599 -603

The electronic properties of 1, 5-diamino-tetrazole (DAT) and isomerization reaction kinetics were studied based on density functional theory.

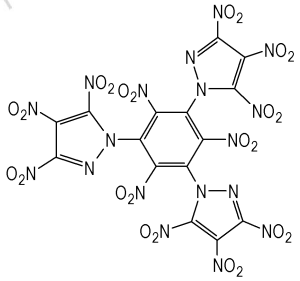
Selection of Carbon Phase in Calculation of Detonation Performance by VLWR Program for CHNO Explosives

WEI Xian-feng, LONG Xin-ping, HAN Yong

Chinese Journal of Energetic Materials, 2013, 21(5): 604 -608

With revised VLWR program, the Gibbs free energy of graphite, diamond and liquid carbon were calculated and the most likely carbon phase at CJ point was confirmed based on the minimum Gibbs free energy principle.

Empirical Calculation of the Explosion Parameters of Nitrodiazole Explosives (Ⅱ)



WANG Jun, JING Mei, ZHANG Xiao-yu, MA Qing, LI Jin-shan, SHU Yuan-jie

Chinese Journal of Energetic Materials, 2013, 21(5): 609 -611

New polynitropyrazole explosive molecules were designed with 3,4,5-dinitropyrazole as structural unit, and the explosion parameters of the designed explosive were calculated by empirical equations.

Estimation and Determination of the Solubility Parameter of 1,5-Diazido-3-nitrazapentane

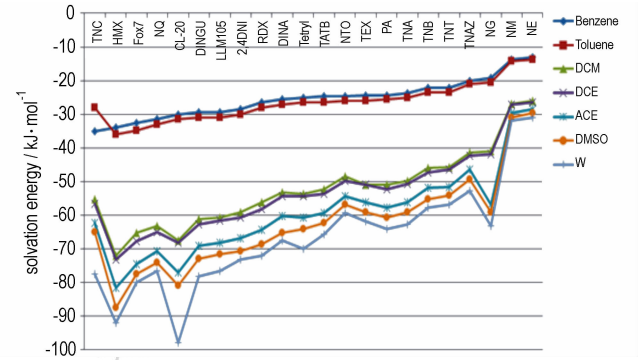
$$\delta = \left(\frac{E}{V}\right)^{1/2} = \left(\frac{\Delta H - RT}{M/d}\right)^{1/2}$$

JI Yue-ping, GAO Fu-lei, HAN Rui, CHEN Bin, WANG Ying-lei, LIU Wei-xiao, LIU Ya-jing, YAO Yi-lun

Chinese Journal of Energetic Materials, 2013, 21(5): 612 -615

The solubility parameter of 1,5-diazido-3-nitrazapentane (DIANP) was estimated by group contribution method and determined by turbidity titration method. The solubility of DIANP in different solvents was studied.

Solvation Effect on Coventional Explosives

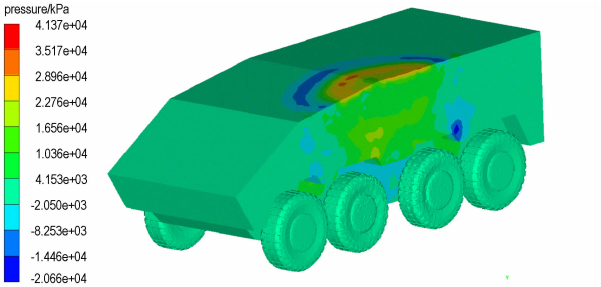


The effects of seven solvents on the feature bond lengths, nitro group charges, dipole moment, solvation energy and bond dissociation energy of 22 common explosives were investigated based on DFT and PCM.

JI Chun-liang, LI Jie, LUO Yun-jun, ZHANG Chao-yang

Chinese Journal of Energetic Materials, 2013, 21(5): 616 −623

Dynamic Response Analysis of an Armored Vehicle under Explosive Loading

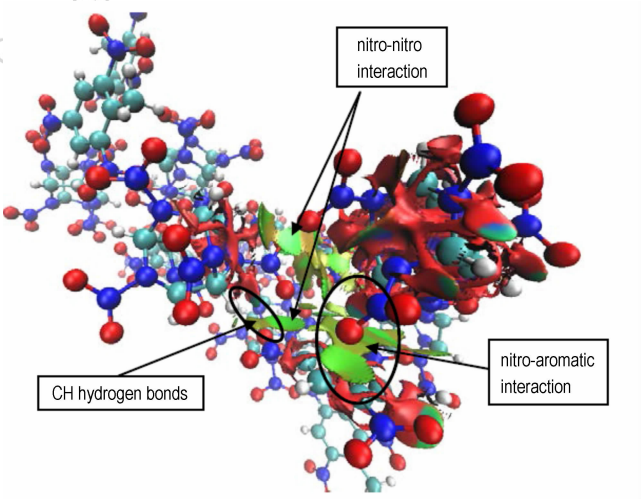


3D simulation of an armored vehicle model composed of 4340 steel and rubber was performed by AUTODYN software. The explosion process of 8701 explosive under different charge mass conditions was calculated. The response parameters of three observation points on the side such as overpressure, displacement and acceleration were obtained. The regularity of dynamic response for the observation points was analyzed.

LU Xiang-hui, ZHOU Chun-gui, WANG Zhi-jun, ZHANG Ming, DUAN Jia-qing

Chinese Journal of Energetic Materials, 2013, 21(5): 624 −628

Progress of Computer Simulation for Intermolecular Interactions in Composite Explosive



Computer simulation methods such as quantum chemistry calculation, molecular mechanics, molecular dynamics and dissipative particle dynamics were introduced.

QIAN Wen, SHU Yuan-jie

Chinese Journal of Energetic Materials, 2013, 21(5): 629 −637

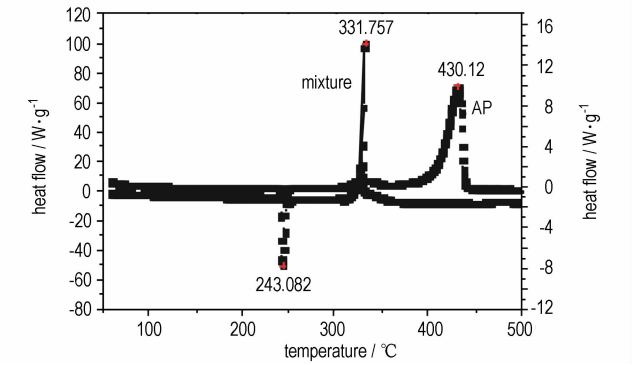
Study on Inclusion of Unstable Energetic Material 1-Amino-1-hydrazino-2,2-dinitroethylene

ZHAO Dong-mei, ZHANG Guo-fang, BI Fu-qiang, FAN Xue-zhong, ZHAO Feng-qi

Chinese Journal of Energetic Materials, 2013, 21(5): 638 −643

The inclusion behaviors of 1-amino-1-hydrazino-2, 2-dinitroethylene (AHDNE) using *p*-tertbutylcalix[*n*]arenes(*n* = 4, 6, 8) and *β*-cyclodextrin as well as their nitration derivatives were investigated. The stability constants and host-guest ratios of the inclusion compounds were calculated and the sensitivity of an inclusion complex was determined.

Synthesis and Properties of TANPyO and its Metal Complexes

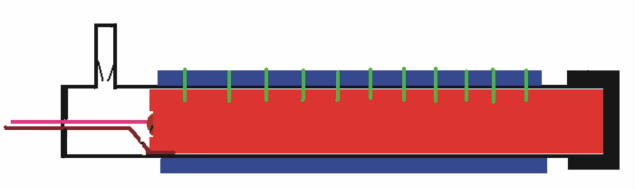


LIU Jin-jian, LIU Zu-liang, LIN Xiang-yang, CHENG Jian, FANG Dong

Chinese Journal of Energetic Materials, 2013, 21(5): 644 −648

Two transition metal complexes with ligand 2, 4, 6-triamino-3, 5-dinitropyridine-1-oxide (TANPyO) were synthesized. Thermal decomposition processes and the catalytic performance toward thermal decomposition of AP were explored.

Deflagration to Detonation Transition Characteristics for Heated PBX-2

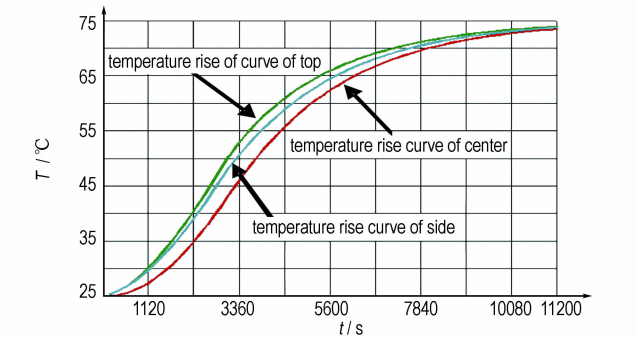


DAI Xiao-gan, Wang Juan, WEN Yu-shi, Huang Yi-min, DAI Ming-hong

Chinese Journal of Energetic Materials, 2013, 21(5): 649 −652

The deflagration to detonation transition (DDT) test loading system for heated explosive was designed. The processes of temperature changing for device shell and explosive were measured by thermocouples. The transmitting time and distance were analyzed by ionic probe. The characteristic of DDT for unheated and heated explosives were obtained.

Detonation Performance of TATB Based PBX at 75 ℃

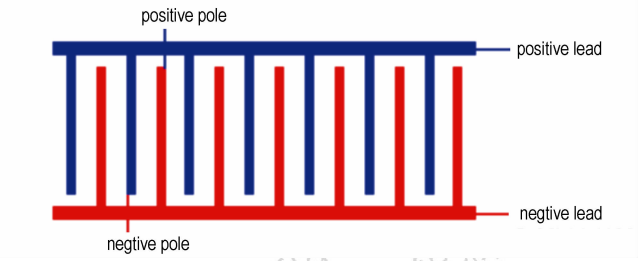


TU Xiao-zhen, LI Wei, WEI Xing-wen, LU Xiao-jun

Chinese Journal of Energetic Materials, 2013, 21(5): 653 −655

The sensitivity to shock wave, detonation velocity, detonation pressure and power of TATB based PBX at 25 ℃ and 75 ℃ were tested by standard scale gap test, electrometric method, standardization method, ZWB253 −2008 and cylinder test.

Experimental Study on Flying Laws Detonation Driven Precast Fragments by Comb Targets Method

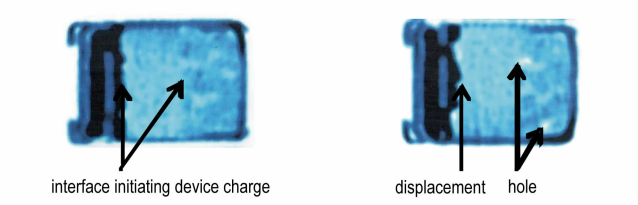


YANG Gui-hong, WANG Guang-jun, GONG Yan-qing, SUN Yong-qiang

Chinese Journal of Energetic Materials, 2013, 21(5): 656 −659

Flying velocities of pre-made fragments (tungsten alloy) were measured by comb targets method. The experimental results of flying law and long distance flying time are agreement with laser measurement method.

Performance of Stab Delay Initiating Device under Overload Shock

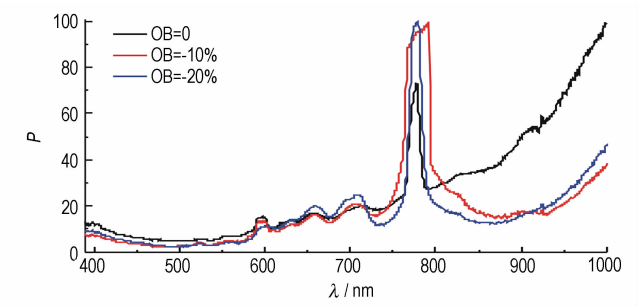


ZHANG Zhou-mei, WANG Pei-yong, SHEN Yi-lin, ZHANG Ye, WANG Guo-qiang, JIA Yu-xin, XU Shuan-lao, FAN Long-long

Chinese Journal of Energetic Materials, 2013, 21(5): 660 −663

The performance of stab delay initiating device affected by overload shock was studied by Split Hopkinson Pressure Bar (SHPB) test. Structural damage of stab delay initiating device was analyzed by CT.

Combustion Spectra of Pyrotechnic Composites Containing Rare-Earth Elements



LI Xue-jun, CONG Xiao-min, DU Zhi-ming, ZHAO Jia-yu

Chinese Journal of Energetic Materials, 2013, 21(5): 664 −667

Relative radiant power distributions of pyrotechnic composites containing rare-earth elements were studied by a transient spectral radiometer. The spectral properties were analyzed from the spectrogram.

Review on Energetic Nitroguanidine Derivatives

ZHANG Guang-quan, LIU Xiao-bo, HUANG Ming

Chinese Journal of Energetic Materials, 2013, 21(5): 668 −674

Synthesis methods of energetic nitroguanidine (NQ) derivatives were reviewed. The performance of some compounds in these energetic NQ derivatives was introduced.

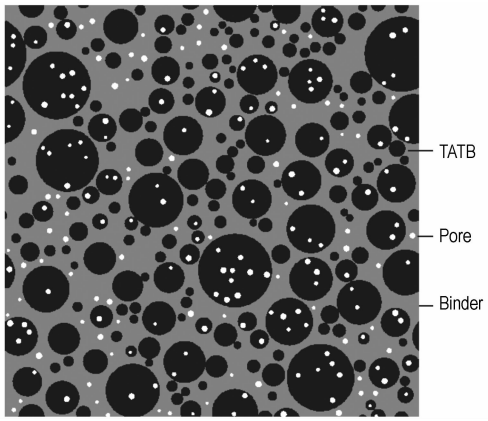
Review on Dynamical Mechanical Properties of Propellants

CHEN Yan-kun, LUO Xing-bai, ZHEN Jian-wei, ZHANG Yu-ling

Chinese Journal of Energetic Materials, 2013, 21(5): 675 −680

Application status of drop weight impact test, air gun test, split Hopkinson pressure bar test and dynamic extrusion physical simulation test in study of dynamical mechanical properties of propellant were introduced. The progress of dynamical mechanical properties of propellant was reviewed with 50 references.

Numerical Simulation of the Porosity Influence on Thermal Conductivity of Polymer Bonded Explosive

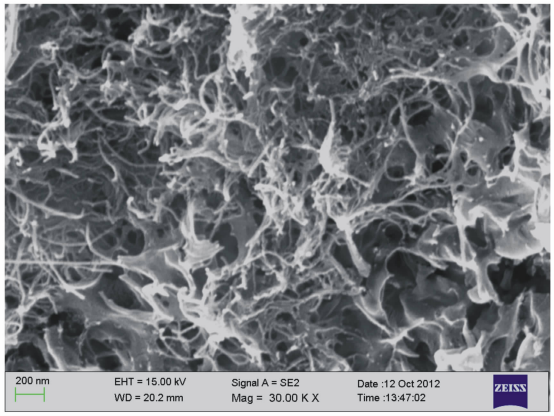


WEI Xing-wen, LI Ming, ZHOU Xiao-yu, HUANG Zhong

Chinese Journal of Energetic Materials, **2013**, **21**(5): **681 −683**

A representative volume element (RVE) model was developed to investigate the effective thermal conductivity of three-phase polymer bonded explosive (PBX).

Improvement of Antistatic Ability of Nitrocellulose

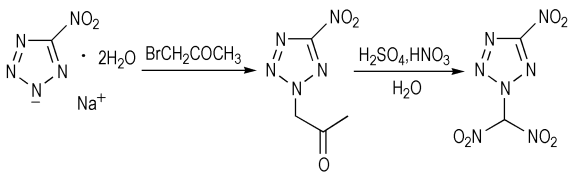


LI Yi, LI Zhao-qian, HUANG Hong-chi, PEI Chong-hua

Chinese Journal of Energetic Materials, **2013**, **21**(5): **684 −687**

A kind of antistatic nitrocellulose membrane was prepared by adding conductive filler to the nitrocellulose. Scanning electron microscope images reveal that some interlaced conductive networks were formed, which result in the electrostatic dissipation. Compared with unmodified nitrocellulose, the surface resistivity and volume resistivity of the membrane reduce by 6 orders of magnitude and 3 orders of magnitude respectively and the electrostatic spark sensitivity increases by 14%.

Synthesis and Properties of 2-Dinitromethyl-5-nitrotetrazole

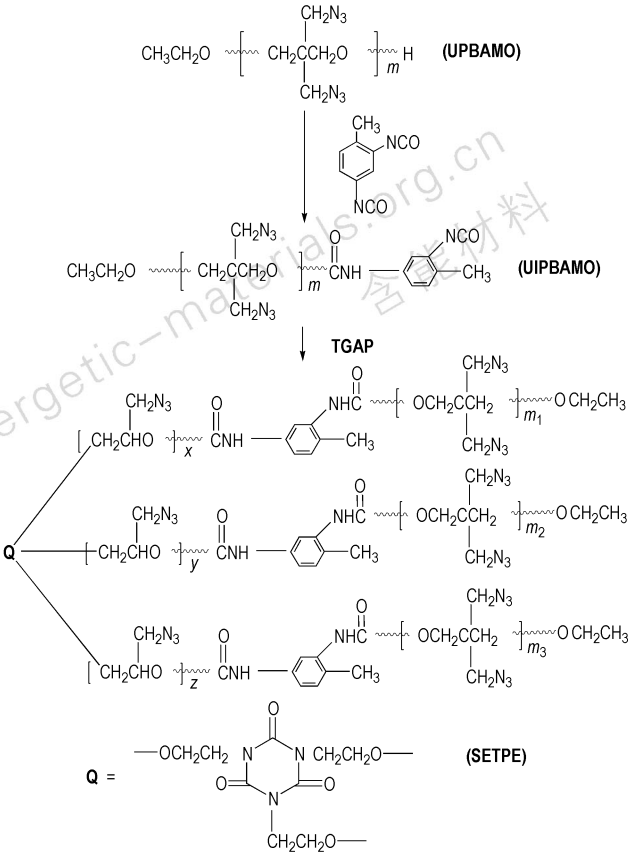


ZHANG Min, GE Zhong-xue, BI Fu-qiang, XU Cheng, LIU Qing, LI Tao-qi

Chinese Journal of Energetic Materials, **2013**, **21**(5): **688 −690**

2-Dinitromethyl-5-nitrotetrazole (HDNMNT) was synthesized via the reactions of substitution and nitration-hydrolysis. The density, enthalpy of formation and detonation parameters were calculated theoretically, and the thermal stability was analyzed by DSC method.

Synthesis and Properties of A_nB Star ETPE Based on PBAMO/TGAP

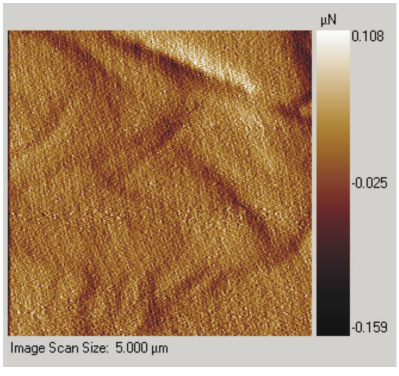


A novel A_nB star energy thermoplastic elastomers (SETPE) based on poly(3,3-bis-azidomethyl oxetane) (PBAMO)/trifunctionality glycidyl azide polymer (TGAP) was prepared via a urethane reaction of functional prepolymers, using unifunctionality PBAMO (UPBAMO) as hard blocks, TGAP as soft blocks, tolyene 2,4-diisocyanate (2,4-TDI) as linking compound. The product was characterized by FTIR, ^{1}H NMR and ^{13}C NMR and GPC.

ZHANG Zhi-gang, LU Xian-ming, MO Hong-chang, LI Lei, YAO Yi-lun, LIU Ya-jing

***Chinese Journal of Energetic Materials*, 2013, 21(5): 691 −692**

Precision Machining of RDX Single Crystal



Cyclotrimethylene trinitramine (RDX) single crystal prepared from acetone solution by solvent evaporation was precision processed by cutting, grinding and polishing, and its root mean squared roughness of the surface was less than 5 nm.

ZHOU Xiao-qing, LI Hong-zhen, LIU Jia-hui, ZHANG Qi, XU Rong, YANG Zong-Wei, LAN Lin-gang

***Chinese Journal of Energetic Materials*, 2013, 21(5): 693 −695**

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