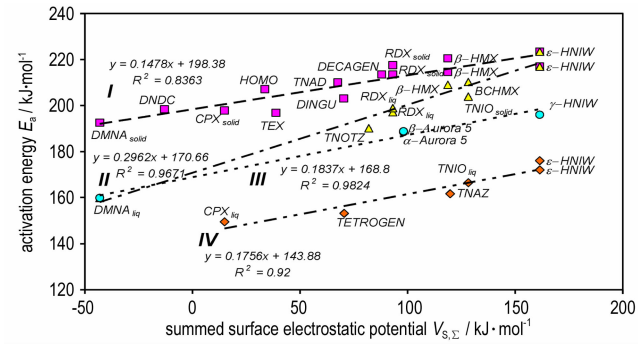
Comparison with Molecular Surface Electrostatic Potential and Thermal Reactivity of Nitramines

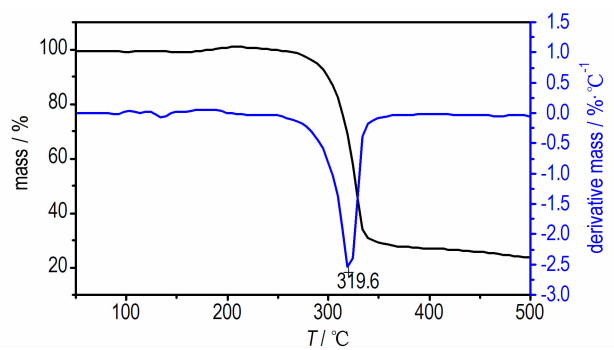


Molecular surface electrostatic potentials $V_S(r)$ (ESP) of seventeen nitramines have been calculated. As a criterion of the imbalance between the $V_{S,max}$ and $V_{S,min}$ extremes their sum was derived and used as a new simple characteristic for ESPs-$V_{S,\Sigma}$. These $V_{S,\Sigma}$ values have close relationships with the Arrhenius parameters, E_a and log$A$, of thermal decomposition of the nitramines studied. The correlation between the $V_{S,\Sigma}$ values and heats of fusion of the nitramines studied is described.

Svatopluk Zeman, Zdeněk Friedl, Monika Bartošková, Qi-Long YAN

Chinese Journal of Energetic Materials, 2015, 23(12): 1155–1161

An Energetic Pb(Ⅱ) Complex of TANPyO: Synthesis, Thermal Decomposition Behavior and Catalytic Effect on Thermal Decomposition of AP

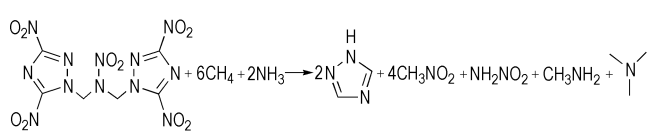


An energetic Pb(Ⅱ) complex of TANPyO was synthesized, and its structure and properties were characterized with FT-IR spectroscopy, elemental analysis, sensitivity tests, TG-DTG and DSC.

CHENG Jian, ZHANG Rong-xian, FU Dai-xuan, ZHAO Feng-qi, XU Si-yu, WANG Xiao-min, LIU Zu-liang

Chinese Journal of Energetic Materials, 2015, 23(12): 1162–1166

Synthesis and Properties of *N*, *N*-Bis((3,5-dinitro-1*H*-1,2,4-triazol-1-yl)methyl) nitramine

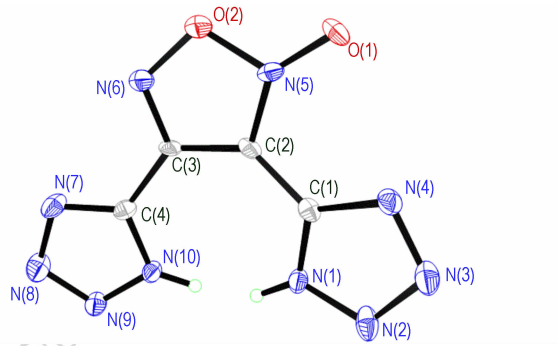


N, *N*-bis((3, 5-dinitro-1*H*-1, 2, 4-triazol-1-yl) methyl) nitramine (BDNTMN) was synthesized via diazotization, nitration and *N*-alkylation etc reactions using 3,5-diamino-1,2,4-triazole (DAT) as starting material. The structures of each compound were characterized by means of ^{1}H NMR, ^{13}C NMR, IR, MS and elemental analysis. The thermal behaviors of BDNTMN were analyzed by DSC and TG. The physicochemical property and detonation performance of BDNTMN were predicted by Gaussian 09 and Kamlat-Jacbos equations.

LI Ya-nan, WU Min-jie, ZHANG Sheng-yong, LIU Ning, WANG Bo-zhou

Chinese Journal of Energetic Materials, 2015, 23(12): 1167–1171

Facile Synthesis and Crystal Structure of 3,4-Bis(1*H*-5-tetrazolyl)furoxan

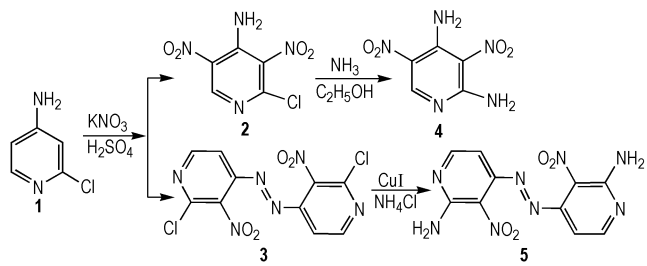


ZHAI Lian-jie, FAN Xue-zhong, WANG Bo-zhou, BI Fu-qiang, HUO Huan, LI Ya-nan, LI Xiang-zhi

Chinese Journal of Energetic Materials, 2015, 23(12): 1172–1175

3,4-Bis(1*H*-5-tetrazolyl)furoxanwas easily synthesized from 3,4-dicyanofuroxan. The single crystal of the compound was studied by X-ray single-crystal diffraction.

Synthesis and Characterization of Two New Energetic Polyamino and Nitro Pyridine Derivatives

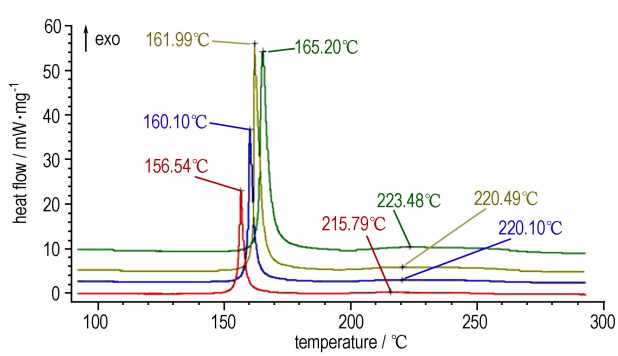


MA Cong-ming, LIU Zu-liang, YAO Qi-zheng

Chinese Journal of Energetic Materials, 2015, 23(12): 1176–1180

A newazo-bridged pyridine derivative (*E*)-1,2-bis(2-chloro-3-nitropyridin-4-yl) diazene (**3**) and 2-chloro-4-amine-3,5-dinitropyridine (**2**) were synthesized through a direct nitration reaction using 2-chloro-4-aminopyridine(**1**) as a primary material, followed by a simple amination reaction to give (*E*)-1,2-bis(2-amino-3-nitro-pyridin-4-yl) diazene(**5**) and 2,4-diamino-3,5-dinitropyridine(**4**).

Non-isothermal Decomposition Kinetics, Specific Heat Capacity and Adiabatic Time-to-explosion of Cu(pn)$_2$(FOX-7)$_2$



GONG Xiang, SUN Qian, XU Kang-zhen, SONG Ji-rong, ZHAO Feng-qi

Chinese Journal of Energetic Materials, 2015, 23(12): 1181–1185

Thermal decomposition of Cu(pn)$_2$(FOX-7)$_2$(pn = 1,3-diaminopropane) was studied.

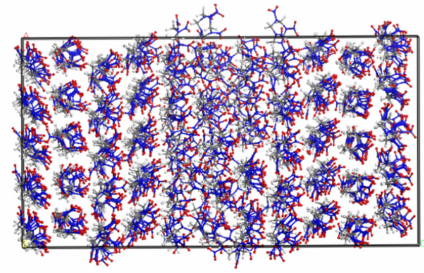
Impact Sensitivity in Respect of the Crystal Lattice Free Volume and the Characteristics of Plasticity of Some Nitramine Explosives

Svatopluk Zeman, Marcela JUNGOVÁ, Qi-Long YAN

Chinese Journal of Energetic Materials, 2015, 23(12): 1186–1191

The relationship between the crystal lattice free volume, ΔV, and impact sensitivity, E_{dr}, of ten nitramines has been analyzed. Also, relationships between the E_{dr} values, on the one hand, and bulk modulus, K, and shear modulus, G, on the other, have been discussed.

Molecular Dynamics Simulations of Crystalline δ-HMX with Void Defect

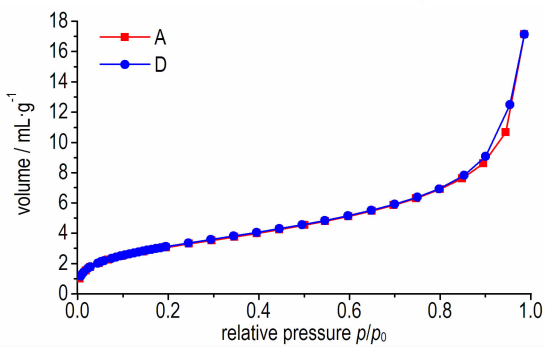


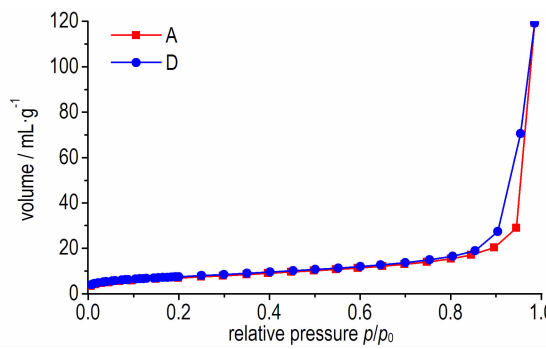
LIAO Ning, LI Wen-peng, ZHOU Xiao-qing, DUAN Xiao-hui

Chinese Journal of Energetic Materials,2015,23(12):1192–1197

The void defect evolvement and molecular conformational transition in crystalline δ-HMX were simulated applying molecular dynamics (MD) method and a compared research with β phase was performed.

Microstructure and Fractal Characteristics of Superfine TATB and HNS



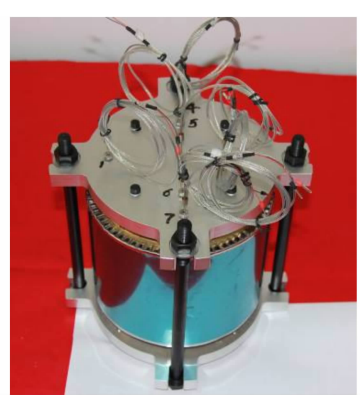


YU Wei-fei, LIAO Long-yu, CHEN Ya, YANG Guang-cheng, LI Jin-shan

Chinese Journal of Energetic Materials,2015,23(12):1198–1201

Microstructures and fractal characteristics of two superfineexplosives conglomeration were researched.

Response Characteristics of PBX-6 Explosive in Slow Cook-off Tests

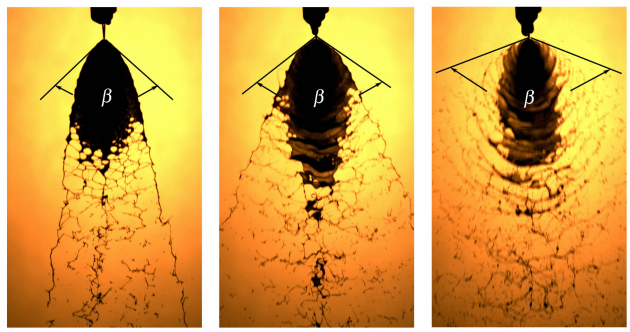


CAO Luo-xia, CAO Wei, WEN Shang-gang, SHEN Chun-ying, CHEN Liang-jun, ZHOU Jian-hua, GAO Da-yuan

Chinese Journal of Energetic Materials,2015,23(12):1202–1206

The devicewas designed for the slow cook-off tests of SR50 mm explosive sphere, and slow cook-off tests with heating rates of 2 ℃ · min^{-1} and 5 ℃ · min^{-1} were carried out respectively. Through analysis of the temperature histories, the shock wave overpressure and the residues after deflagration, the safety of PBX-6 explosive components under slow heating conditions was evaluated.

Atomization of Gelled Propellant Simulant with Carbon Particles

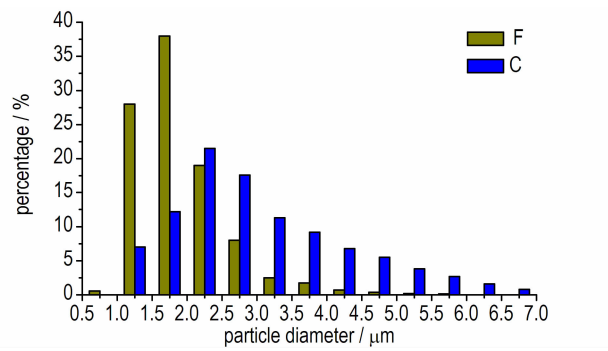


QIANG Hong-fu, LIU Hu, HAN Qi-long, WANG Guang, HAN Ya-wei

Chinese Journal of Energetic Materials, 2015, 23(12): 1207–1211

Atomization characteristics of a gelled propellant simulant with 5% carbon particles with an average diameter of about 5 μm were investigated.

Applicability of Two Kinds of Micromixers for High Viscosity Fluid Emulsification Process

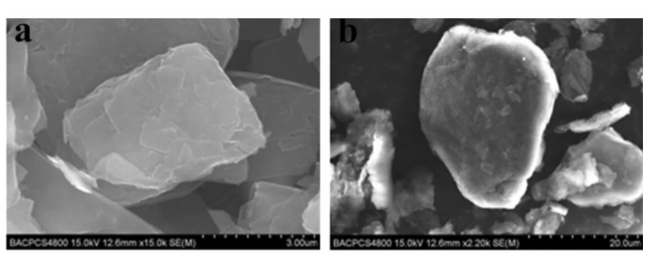


WANG Kai, LIU Da-bin, QIAN Hua, XU Sen, LI Chang-hong, LI Xue-fei

Chinese Journal of Energetic Materials, 2015, 23(12): 1212–1216

Two types of micromixers were used to complete separately the first emulsification and the second emulsification of emulsion matrix. Both of the emulsion principle of the split-recombine micromixer for high viscosity fluid and the influence of the width, length of the microchannel and fluid flow velocity on the emulsification effect were discussed.

Flowability and Infrared Interference Properties of Modified Graphite Flake with Hydrophobic Nano-silica

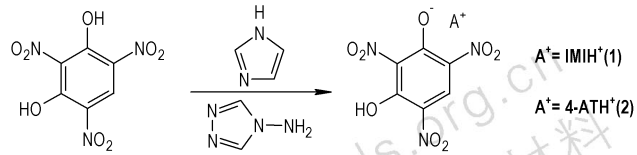


NING Gong-tao, LI Ping, CUI Yu-ling, LI Shi-chuan, TANG Run-ze, ZHOU Zun-ning

Chinese Journal of Energetic Materials, 2015, 23(12): 1217–1220

The flowability of graphite flake particles before and after modification was measured by a powder property tester. The smoke was formed by dispersing the graphite flake particles into the smoke box using air flow dispersion way. The mass concentration and IR spectrum transmission of the smoke were measured. The settling velocity of smoke was calculated.

Two new Energetic Ionic Salts with Environmental Protection: Preparation and Thermal Properties of IMI·TNR and 4-AT·TNR

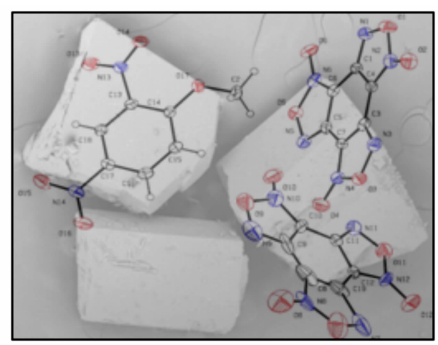


LI Ying, BI Yan-gang, ZHAO Wen-yuan, GUO Wei-ming, ZHANG Tong-lai

Chinese Journal of Energetic Materials, 2015, 23(12): 1221–1227

Two environmental friendly energetic salts were prepared from styphnate with imidazolium (IMI), 4-amino-1, 2, 4-triazolium(4-AT) under normal conditions. Their structures were characterized by IR, elemental analyses and X-ray single crystal analysis.

Preparation and Performance of BTF-DNAN Cocrystal Explosive

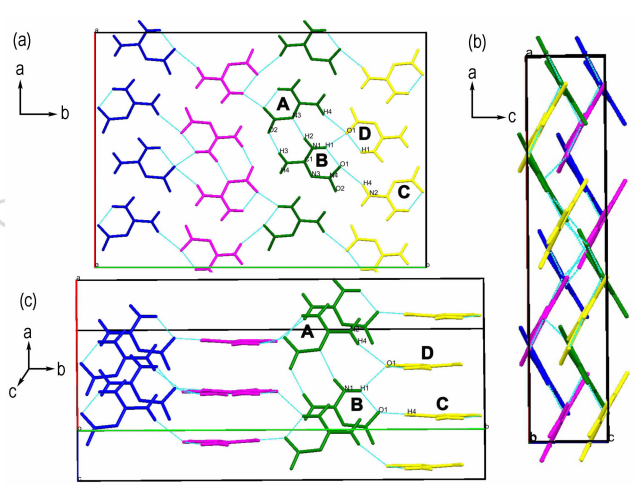


MA Yuan, HAO Shi-long, LI Hong-zhen, LIU Yu-cun, YANG Zong-wei

Chinese Journal of Energetic Materials, 2015, 23(12): 1228–1230

A novel energetic cocrystal composed of benzotrifuroxan (BTF) and 2,4-dinitroanisole (DNAN) in a 2∶1 molar ratio was synthesized by solvent evaporation.

Anisotropic Thermal Expansion in Nitroguanidine Crystal

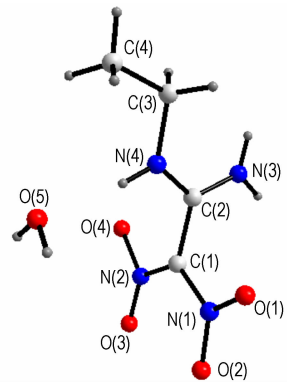


ZHANG Hao-bin, XU Jin-jiang, LI Jing-you, LIU Yu, LIU Xiao-feng, SUN Jie

Chinese Journal of Energetic Materials, 2015, 23(12): 1231–1234

Highlyanisotropic and negative thermal expansion in nitroguanidine crystal caused by a shrink of crystal along the *b* axis with the enlargement of intermolecular distances and decrease of space hindrance as temperature increase are reported.

Crystal Structure and Enthalpy of Combustion of AEFOX-7

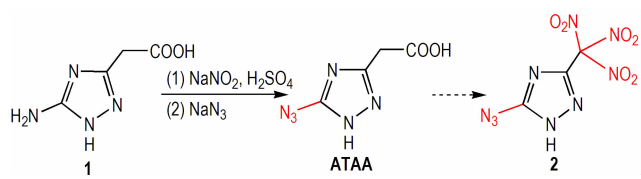


SUN Qian, LI Yan-feng, XU Kang-zhen, SONG Ji-rong, ZHAO Feng-qi

Chinese Journal of Energetic Materials, 2015, 23(12): 1235–1239

The single crystal of 1-amino-1-ethylamino-2,2-dinitroethylene monohydrate (AEFOX-7 · H_2O) was obtained. The enthalpies of combustion of AEFOX-7, AMFOX-7 (1-amino-1-methylamino-2,2-dinitroethylene) and FOX-7 at 298.15 K were determined.

Synthesis and Thermal Behavior of 5-Azido-1, 2, 4-triazolyl-5-acetic Acid (ATAA)



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

Chinese Journal of Energetic Materials, 2015, 23(12): 1240–1242

A novel azido-triazole, 5-azido-1,2,4-triazolyl-5-acetic acid(ATAA), was synthesized for the first time by Sandmeyer-Reaction in a mixed system (including sodium nitrite, sulfuric acid and sodium azide).

The Empirical Nitrogen Equivalent Equations for Predicting the Detonation Velocity and Detonation Pressure of CHNO Explosives with Approaching the Results of Kamlet-Jacobs Equations

$$D=\frac{100}{M}(695+1150\rho)\ (1.00x_{N_2}+0.64x_{H_2O}+1.34x_{CO_2}+0.72x_{CO}+0.18x_{H_2}+0.50x_{O_2}+0.12x_C)$$

$$p=1.060\left[\rho\frac{100}{M}(1.00x_{N_2}+0.64x_{H_2O}+1.34x_{CO_2}+0.72x_{CO}+0.18x_{H_2}+0.50x_{O_2}+0.12x_C)\right]^2-0.619$$

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

Chinese Journal of Energetic Materials, 2015, 23(12): 1243–1262

Two empirical nitrogen equivalent equations for predicting the detonation velocity (D) and detonation pressure (p) of CHNO explosives with more approaching the values of D and p in Kamlet-Jacobs equations than common used nitrogen equivalent equations were presented.
