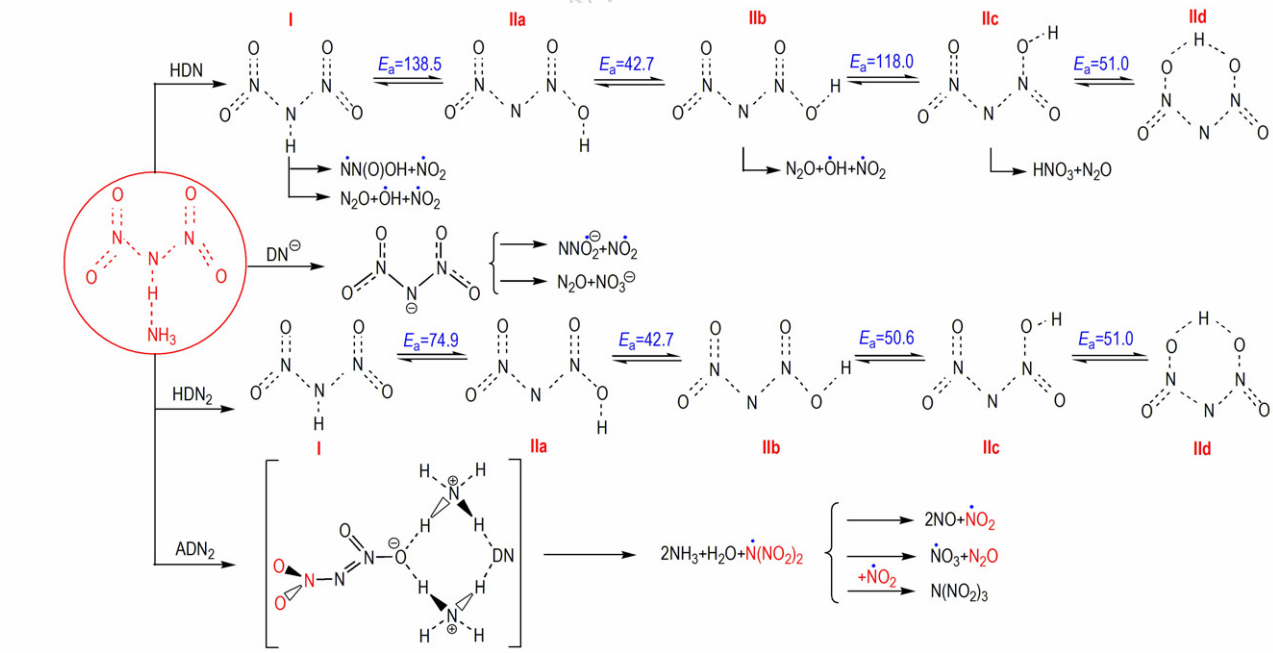
Derived Ways of the Rate Equations of Autocatalytic Reaction and Their Application in Thermal Behavior Study of Energetic Materials

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

Chinese Journal of Energetic Materials,2015,23(9): 818–830

The kinetic parameters, rate curve characteristic parameters and the equation of change in reaction extent with time for the autocatalytic decomposition reaction of hexanitrohexaazaisowurtzitane (HNIW) and nitrocellulose (NC) (12.82%, 12.97%, 13.54%, 13.61%, 13.88%, 14.14% N) and the derived ways of equations used in calculation of these parameters were reported.

Review on Theoretical Investigations of the Thermal Decomposition of Ammonium Dinitramide

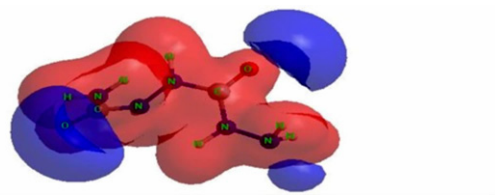


Proposed possible mechanism of proton transference and decomposition reaction in the different models of ADN, in which the main decomposition reactions, products and active energies (in kJ·mol^{-1}) of ADN, to a certain extent can be explained.

WANG Zhi-yin, XU Qiong, ZHANG Tian-lei, WANG Rui

Chinese Journal of Energetic Materials,2015,23(9): 831–841

Theoretical and Experimental Study of Nitrogen-rich Compounds of Biurea and 1-Amino-biurea

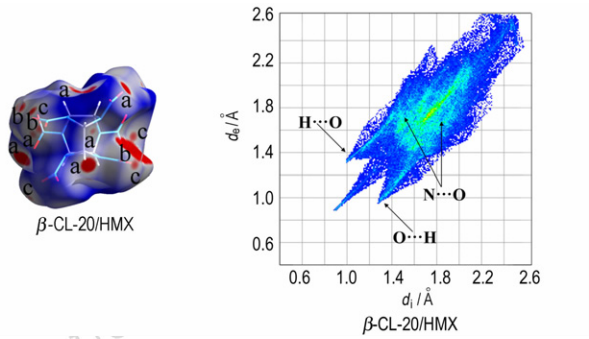


The single crystal of1-amino-biurea was obtained by slow evaporation method in solvent and its structure was determined using X-ray single crystal diffraction. The charge distribution, natural bond orbit and molecular electrostatic potential of biurea and 1-amino-biurea were calculated to study their electronic structural and properties by DTF- B3LYP method with the cc-pVTZ basis set.

WU Jin-ting, ZHANG Jian-guo, NIU Xiao-qing, ZHANG Tong-lai

Chinese Journal of Energetic Materials,2015,23(9): 842–847

Theoretical Research on Packing Structures of Energetic Cocrystals

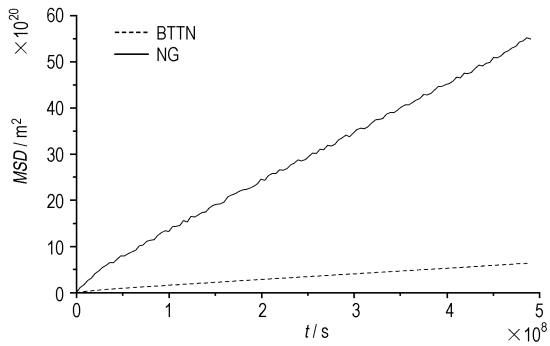


ZHANG An-bang, CAO Yao-feng, MA Yu, ZHU Yuan-qiang, ZHANG Chao-yang

Chinese Journal of Energetic Materials, 2015, 23(9): 848–857

Packing structures of CL-20, HMX, BTF and TNT cocrystals were studied by Hirshfeld surface and fingerprint plot from densities, packing coefficients and molecular interaction contributions.

Mesoscopic Molecular Simulation of Migration of NG and BTTN in Polyurethane

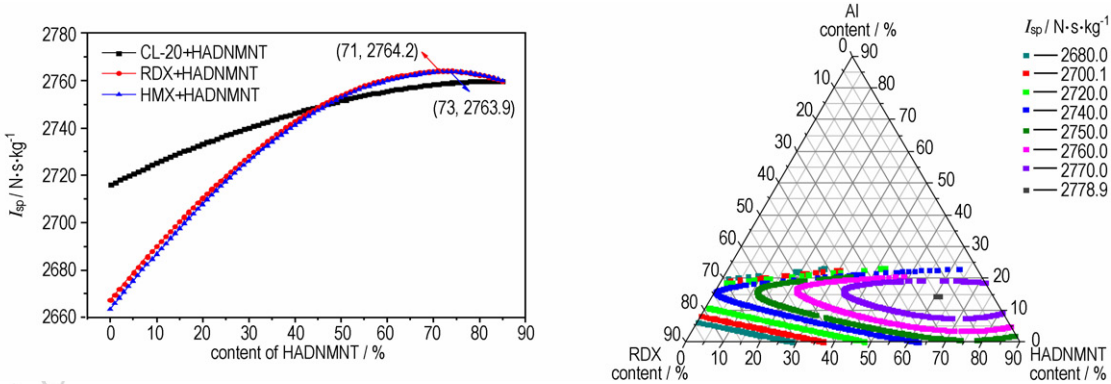


YU Zhen-fei, FU Xiao-long, YU Hong-jian, QIN Guang-ming, TAN Hui-min, CUI Guo-liang

Chinese Journal of Energetic Materials, 2015, 23(9): 858–864

Dissipative particle dynamics method was used to simulate migration of NG and BTTN in polyurethane elastomer.

Computational Investigation of Energy Characteristics of Propellant Containing Hydroxylammonium 2-Dinitromethyl-5-nitrotetrazolate

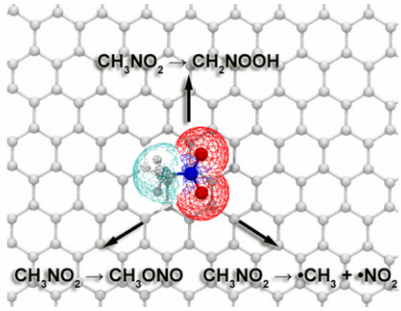


ZHANG Min, BI Fu-qiang, XU Cheng, LIU Qing, GE Zhong-xue, WANG Bo-zhou, WANG Wei, ZHU Yong

Chinese Journal of Energetic Materials, 2015, 23(9): 865–870

The energy parameters of HTPB and CMDB propellants containing hydroxylammonium 2-dinitromethyl-5-nitrotetrazole (HADNMNT) were calculated by minimum free energy method under the standard condition (ratio of chamber pressure to exit pressure (p_c : p_e) is 70/1) and the results show that HADNMNT is a potential high energy material in HTPB and CMDB propellants.

Reaction Mechanism of Nitromethane on the Graphene Surface: A Theoretical Study

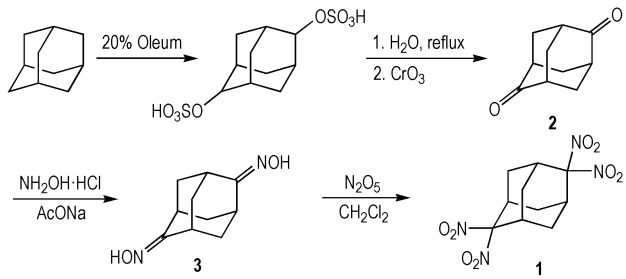


LIU Ying-zhe, KANG Ying, LAI Wei-peng, YU Tao, GE Zhong-xue

***Chinese Journal of Energetic Materials*,2015,23(9): 871–876**

The initial reactions of nitromethane on the graphene surface were studied theoretically, and the corresponding reaction transition states, activation energies, and potential energy surface were obtained.

Synthesis and Characterization of 2,2,6,6-Tetranitroadamantane

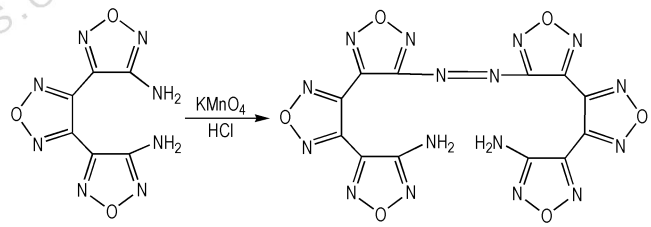


2,2,6,6-Tetranitroadamantane was synthesized by direct oxidative nitration from adamantane-2,6-dionedioxime, which was prepared via oxidation and oximation of adamantane. The structures of the products were confirmed by ^{1}H NMR, ^{13}C NMR, IR and elementary analysis. The reaction conditions of the oxidative nitrition were optimized and the thermal properties of 2,2,6,6-tetranitroadamantane were analyzed by thermogravimetry (TG) and differential scanning calorimetric (DSC) measurements.

LING Yi-fei, SUN Lu, LUO Jun

***Chinese Journal of Energetic Materials*,2015,23(9): 877–881**

Synthesis and Properties of a Novel Energetic Compound 3,3′-Azobis(3-amino-trifurazan)

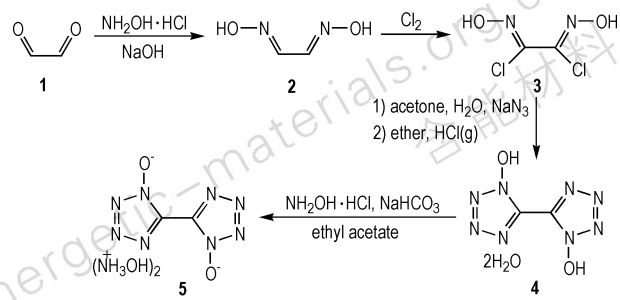


A novel energetic compound 3,3′-azobis(3-amino-trifurazan) (ABATF) was synthesized by oxidation reaction with 3,4-bis(3′-aminofurazan-4′-yl) furazan (BATF) as raw material, and its structure was confirmed by IR, ^{1}H NMR, ^{13}C NMR, MS and elemental analysis. The detonation performances were calculated by Gaussian 09 and VLW equation.

JIA Si-yuan, ZHANG Hai-hao, WANG Bo-zhou, HUO Huan, ZHOU Cheng

***Chinese Journal of Energetic Materials*,2015,23(9): 882–886**

Improved Synthesis of TKX-50

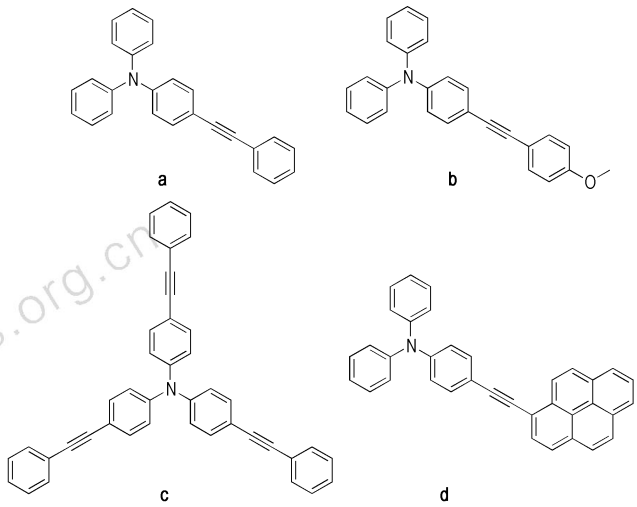


Dihydroxylammonium 1,1′-diolate-5,5′-bistetrazole (TKX-50) was synthesized *via* the reactions of oximation, chloration, azidation-cyclization and neutralization using glyoxal as starting material, and its structure was characterized by NMR, MS, IR. The optimum conditions for azidation-cyclization reaction and neutralization reaction were obtained.

JU Ping-wen, LING Yi-fei, GU Yu-fan, LUO Jun

***Chinese Journal of Energetic Materials*,2015,23(9): 887–891**

Synthesis and Spectral Properties of Alkynyl Substituted Triphenylamines

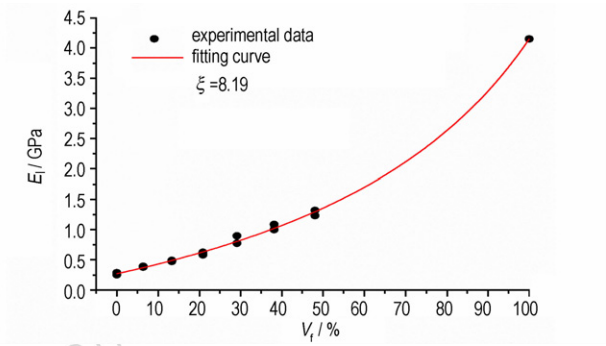


Alkynylsubstituted triphenylamines were synthesized via sonogashira coupling reaction using alkynes and halogenated triphenylamines as raw materials. The effects of molecular structure, solvent polarity, and addition of nitro-explosives on the fluorescent properties were researched.

WANG Shi-chen, JU Jia, AI Wen-tao, YUAN Hao, CAI Hua-qiang, HUANG Hui

***Chinese Journal of Energetic Materials*,2015,23(9): 892–897**

Static Compression Mechanical Properties of RDX Based Aluminum Fiber Explosive

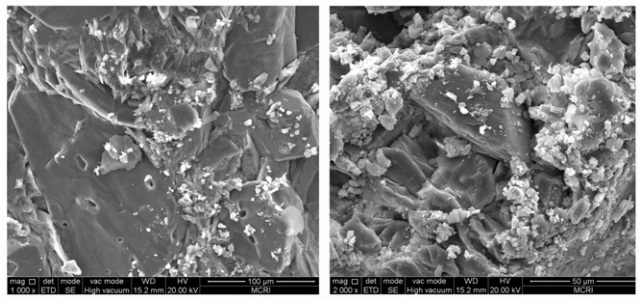


The RDX based aluminum fiber explosive was prepured by replacing aluminum powder in traditional aluminized explosive with aluminum fiber. Quasi-static compression mechanical experiments of the aluminum fiber explosives were carried out.

LIN Mou-jin, CUI Xiao-rong, MA Hong-hao, LI Zhan-jun, JIA Hu

Chinese Journal of Energetic Materials, 2015, 23(9): 898-902

Response Characteristic of JO-8 Explosive and Composition B under Low-speed Impact

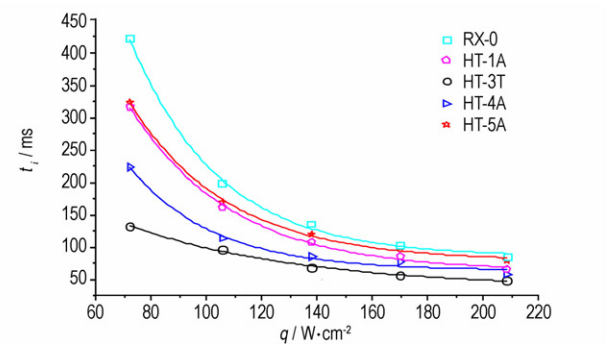


JO-8 and Composition B were investigated by the low-speed impact loading test using the small hammer of 30 kg, and their impacting courses were studied by the high speed photography, and the residue after impacting were analyzed by the scanning electric microscopy.

TIAN Xuan, XU Hong-tao, FENG Xiao-jun, WANG Xiao-feng, NAN Hai, FENG Bo, FENG Xue-song, ZHAO Juan

Chinese Journal of Energetic Materials, 2015, 23(9): 903-907

Laser Ignition Characteristics of AP/HTPB Composite Solid Propellants Containing Metal Nanopowders

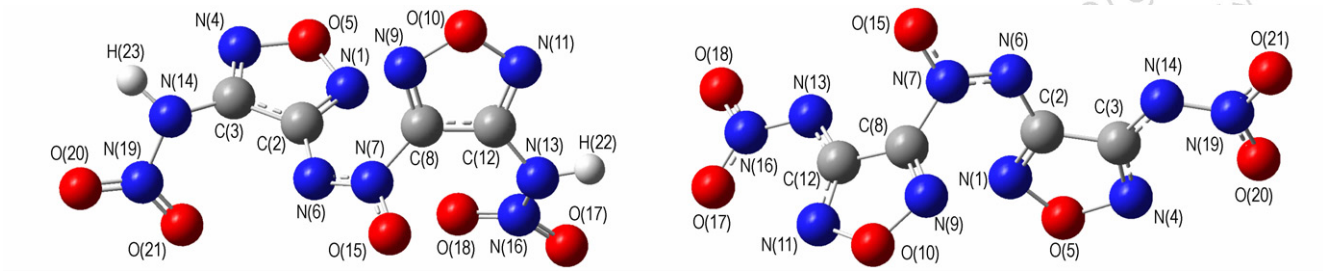


Ignition characteristics of Al micro-powders, Al nanopowders, Ti nanopowder and amine perchlorate (AP)/hydroxyl-terminated polybutadiene (HTPB) composite solid propellants containing metal powders were studied by CO_2 laser ignition method with a wavelength of 10.6 μm at different heat fluxes, and the effects of Al size on ignition characteristics of Al powders and the effect of the different metal powders on ignition characteristics of AP/HTPB composite solid propellants containing metal powders were discussed under heat fluxes from 77.6 W·cm^{-2} to 365.1 W·cm^{-2}.

HAO Hai-xia, YAO Er-gang, WANG Bao-xing, ZHAO Feng-qi, XU Si-yu, PEI Qing

Chinese Journal of Energetic Materials, 2015, 23(9): 908-914

Synthesis and Properties of Two Energetic Salts from 3,3′-Dinitroamino-4,4′-azoxyfurazan



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

***Chinese Journal of Energetic Materials*,2015,23(9): 915–918**

New two kinds of energetic ion salts, carbohydrazide 3,3′-dinitroamino-4,4′-azoxyfurazan (NOF-CBH) and aminoguanidine 3,3′-dinitroamino-4,4′-azoxyfurazan (NOF-AG), were synthesized via metathesis reaction with more nitrogen cation (CBH and AG). The molecular geometry and stability comparison between NOF and its anion (NOF^{2-}) were studied by quantum chemistry calculations.