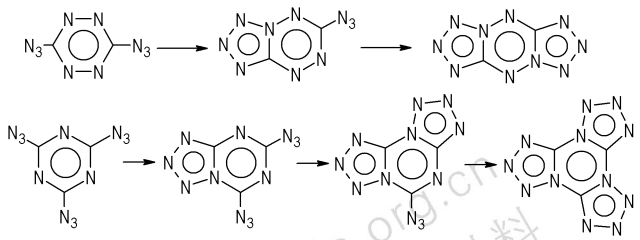
Density Functional Theory Study on Tautomerization of Polyazido-azine

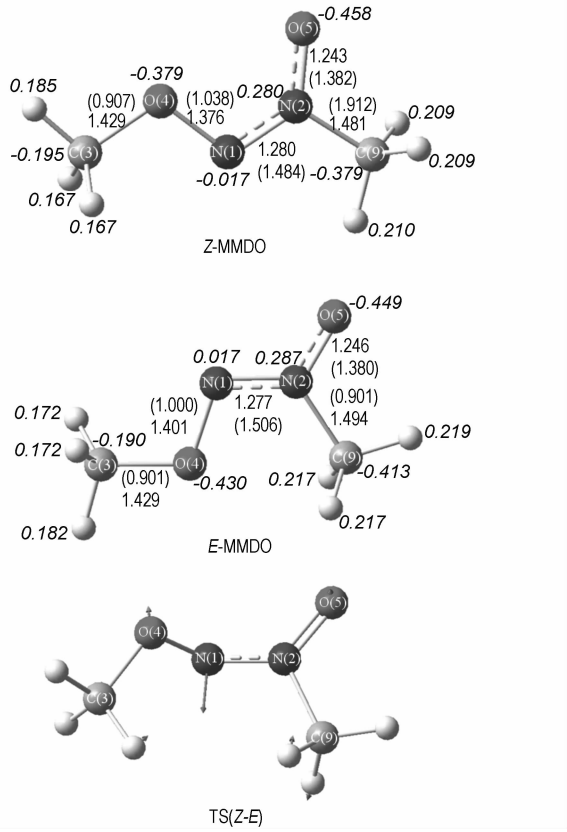


The tautomerizations of polyazido-azine (ring-closure reaction) for 3,6-diazido-1,2,4,5-tetrazine and 2,4,6-triazido-1,3,5-triazine were investigated by density functional theory (DFT) at the B3LYP/6-311G** level.

LI Yu-fang, LIAO Xin, JU Xue-hai, YI Jian-hua, XU Si-yu

Chinese Journal of Energetic Materials, **2010**, **18**(**3**): **241 −246**

Theoretical Study on Structure and Properties of *N*-Methyl-*N*′-methoxydiazene-*N*-oxide



The structure, enthalpy of formation, density and thermal decompostion mechanism of *N*-methyl-*N*′-methoxydiazene-*N*-oxide (MMDO) were studied based on density fuctional theory and compared with its nitramino-isomer dimethylnitramine (DMNA).

XIONG Ying, SHU Yuan-jie, YIN Ming, LONG Xin-ping, ZUO Yu-fen, WANG Xin-feng

Chinese Journal of Energetic Materials, **2010**, **18**(**3**): **247 −251**

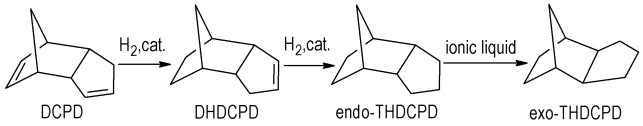
Theoretical Study on Structures and Detonation Performances for Nitro Derivatives of Pyrazole by Density Functional Theory

Nitropyrazole and its derivatives were investigated at the B3LYP/6-311G (d, p) level. And the detonation velocity of the derivatives were estimated between 6.42 and 9.00 km · s^{-1} by the Kamlet-Jacbos equation.

YI Jian-hong, HU Shuang-qi, LIU Sheng-nan, CAO Duan-lin, REN Jun

Chinese Journal of Energetic Materials, **2010**, **18**(**3**): **252 −256**

Synthesis of *Exo*-tetrahydrodicyclopentadiene in Ionic Liquids

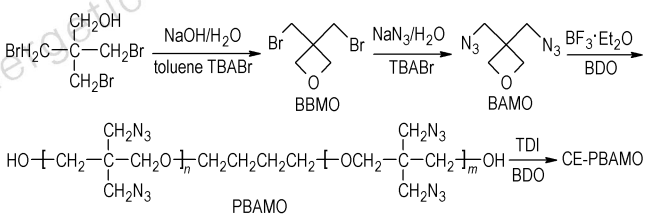


Ionic liquids were prepared by $AlCl_3$ and dialkylimidazolium halide or alkylpyridinium halide and were used in isomerization of *endo*-tetrahydrodicyclopentadiene (*endo*-THDCPD) as catalyst and solvent. The product can be simple separated and ionic liquids can be reused at least five times without decreasing of the catalytic activity.

LI Chun-ying, DU Yong-mei, Lü Jian

***Chinese Journal of Energetic Materials*, 2010, 18(3): 257 −260**

Synthesis of High Energy Thermoplastic Binder CE-PBAMO

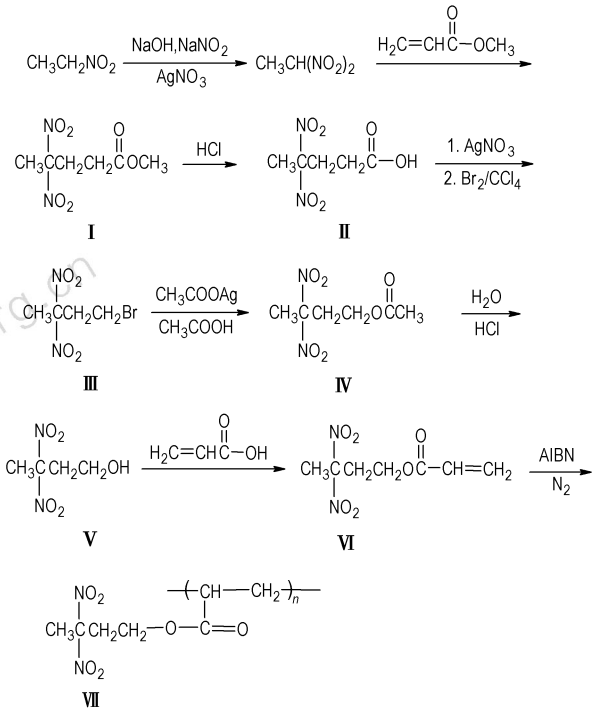


The synthesis of BBMO and BAMO by phase transfer catalysis possesses advantages of safety, high yield and high purity. The synthesized CE-PBAMO can be used as high energy thermoplastic binder in the manufacture of the new type of combustible cartridge case which has concept of 3R(recycle, recover, reuse).

LU Xian-ming, GAN Ning, XING Ying, HAN Tao, LIU Qing, ZHANG Zhi-gang, LI Lei

***Chinese Journal of Energetic Materials*, 2010, 18(3): 261 −265**

Synthesis and Property of Energetic Binder Poly(3,3-dinitrobutyl acrylate)

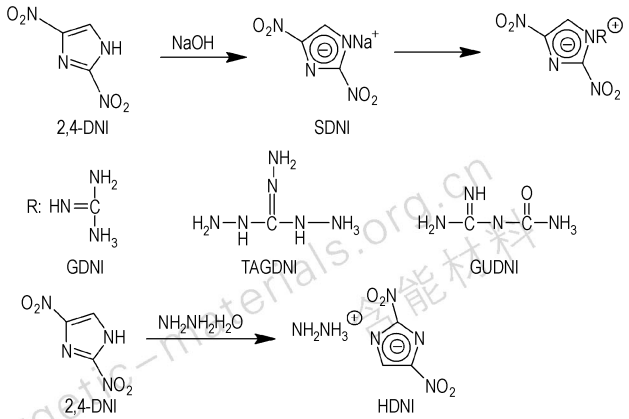


3,3-Dinitrobutyl acrylate was prepared from 3,3-dinitro-1-butanol and acrylic acid through direct esterification, which was obtained by the reaction of six steps using nitroethane as a starting material. The energetic binder poly(3,3-dinitrobutyl acrylate) was synthesized by the free radical polymerization.

ZHANG Gong-zheng, LI Hai-hua, GUO Ling-hong

***Chinese Journal of Energetic Materials*, 2010, 18(3): 266 −269**

Synthesis and Properties of 2, 4-Dinitroimidazole (2,4-DNI) Salts



YANG Wei, JI Yue-ping, WANG Wei,
CHEN Bin, WANG Ying-lei
Chinese Journal of Energetic Materials, **2010**, **18**(3): **270 -272**

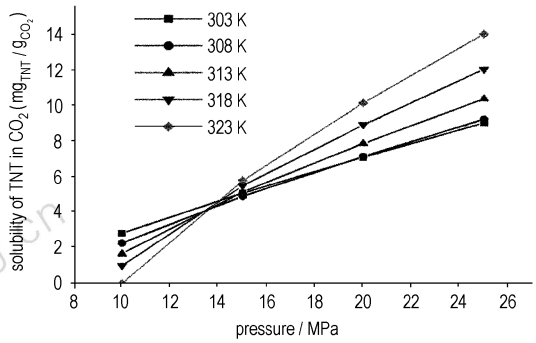
Using 2,4-dinitroimidazole(2,4-DNI) and organic amines as starting materials, four new salts, i. e. ADNI (A = guanidine, triaminoguanidine, gunanyl urea, and hydrazine), were synthesized with yield of 87.2%, 67.5%, 67.7% and 96.6% respectively.

Catalytic Effect of $NiC_2O_4 \cdot 2H_2O$ on Thermal Decomposition of TEGDN/NC Propellant

WEI Wen-xian, JIANG Xiao-hong, LU Lu-de
Chinese Journal of Energetic Materials, **2010**, **18**(3): **273 -277**

$NiC_2O_4 \cdot 2H_2O$ was prepared and characterized by XRD, SEM, laser granularity measurement device, elemental analysis, FT-IR and TG-DTG analysis, and its catalytic effect on the thermal decomposition of TEGDN/NC propellant was analyzed by means of TG-MS.

Solubility of TNT in Supercritical Carbon Dioxide



WEN Li-qun, ZHANG Tong-lai, QIN Qing-feng
Chinese Journal of Energetic Materials, **2010**, **18**(3): **278 -281**

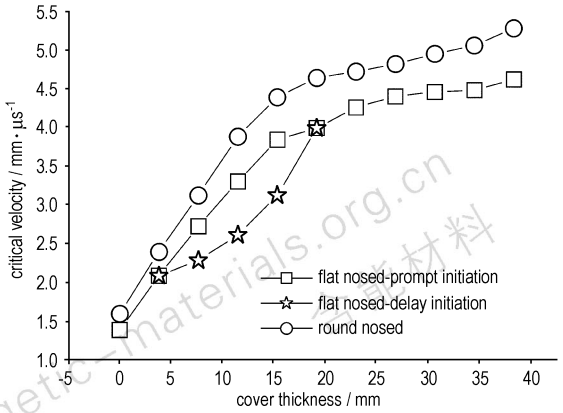
The UV-Vis absorbance data of TNT/acetone, TNT/toluene and TNT/acetonitrile with different concentrations were measured. Acetonitrile was used as recrystallizing solvent, and the solubility of TNT in supercritical carbon dioxide (SC-CO_2) was tested at 303, 308, 313, 318, 323 K and at 10 -25 MPa.

Reaction Behavior for PBX-2 Explosive at Different Heating Rate

DAI Xiao-gan, HUANG Yi-min, Lü Zi-jian, SHEN Chun-ying
Chinese Journal of Energetic Materials, **2010**, **18**(3): **282 -285**

Cook-off tests with different heating rate were carried out for PBX-2 explosive. Reaction law for PBX-2 explosive was analyzed at different heating rate.

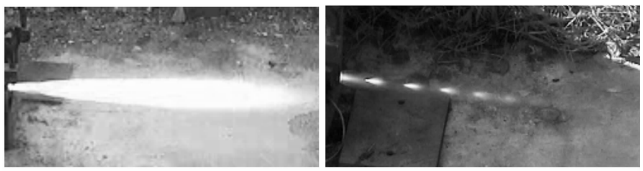
Numerical Simulation of Shock Initiation in Covered Comp B by Projectile Impact



The process of explosion caused by cylindrical flat and round nosed tungsten projectiles impacting the Comp B with various thickness steel cover plates was simulated. The comparison of critical velocity with cover thickness was given.

CUI Kai-hua, HONG Tao, CAO Jie-dong
Chinese Journal of Energetic Materials, **2010**, **18**(**3**): **286 – 289**

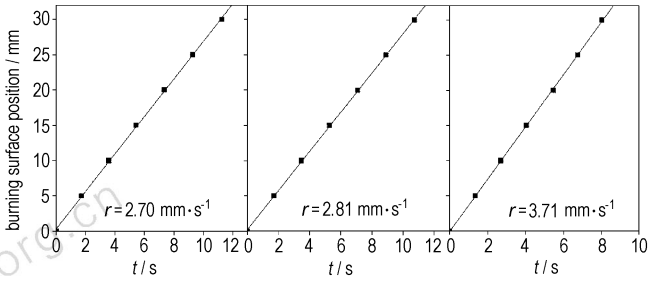
Effect of Performance with Eliminated-flame Additive on Nitramine Modified Double Base Propellant



The motor experiments shown that potassium additives can achieve suppressing exhaust after burning on solid rocket motor.

LI Jun-qiang, LI Xiao-jiang, LIU Peng, QI Xiao-fei, LIU Fang-li
Chinese Journal of Energetic Materials, **2010**, **18**(**3**): **290 – 294**

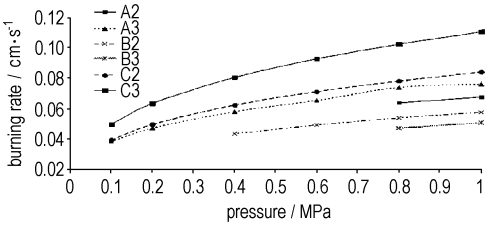
Effects of Oxidants on Combustion Performances of Al/H_2O Based Fuels in Air



Al/H_2O based fuels without additive and with 10% oxidant (HMX or CL-20) were designed and prepared. A series of experiment were carried out to study the effects of the oxidants on the combustion performances of Al/H_2O based fuels in air.

LIN Zhen-kun, HAN Dong-lin, WANG Tian-fang, ZHAO Feng-qi, YI Jian-hua, LI Shu-fen
Chinese Journal of Energetic Materials, **2010**, **18**(**3**): **295 – 299**

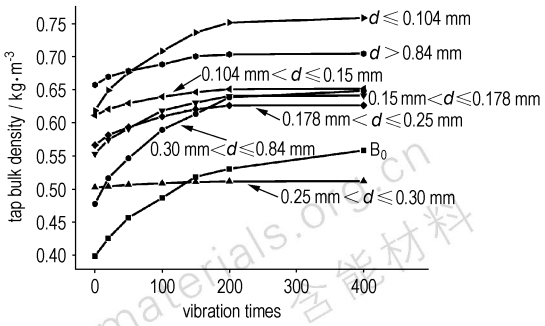
Combustion Behavior of the Low-Smoke Level Fuel-Rich Composite Propellants at Low Pressure



Combustion behavior of composite fuel-rich propellants based on HTPB/AP was studied experimentally at pressure between 0.1 MPa and 1 MPa.

ABDEL WARETH W. M., XU Xu
Chinese Journal of Energetic Materials, **2010**, **18**(**3**): **300 – 303**

Bulk Density of Different Sizes of Agglomerated Boron Particles

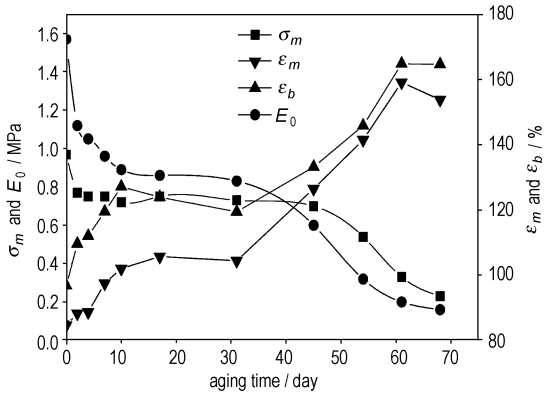


The loose and the tap bulk densities of agglomerated boron particles with different sizes were determined, and the microstructures of agglomerated boron particles were obtained by scanning electrical microscope.

PANG Wei-qiang, FAN Xue-zhong

Chinese Journal of Energetic Materials,2010,18(3): 304 −308

Humidity-heat Combination Stress Aging Behavior of NEPE Propellants



Humidity-heat aging of NEPE propellants can be expressed as a combination of physical aging and thermal aging. The physical aging is in character of humidity aging. And the chemical aging is in character of heat aging. There are cooperative effects in humidity-heat combination stress aging.

CHI Xu-hui, PENG Song, PANG Ai-min,
ZHANG Shi-ping, WU Feng-jun

Chinese Journal of Energetic Materials,2010,18(3): 309 −315

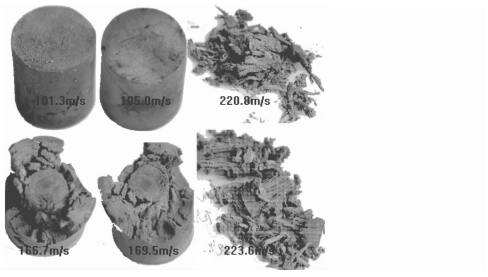
Safety Property of FOX-7 and HTPB Propellants with FOX-7

CHEN Zhong-e, LI Zhong-you, YAO Nan,
LEI Qing, WANG DU

Sensitivities of FOX-7(RDX) and HTPB propellants with FOX-7(RDX) were studied by means of DSC-TG and sensitivity test.

Chinese Journal of Energetic Materials,2010,18(3): 316 −319

Fragility of NEPE Propellant

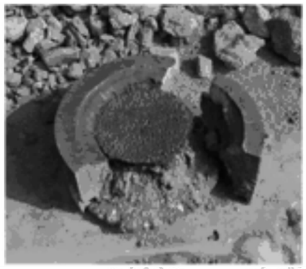


The fragility of NEPE propellant was studied by a simulation device.

LI Jun, ZHAO Xiao-bin, WANG Chen-xue, GUAN Hong-bo

Chinese Journal of Energetic Materials,2010,18(3): 320 −323

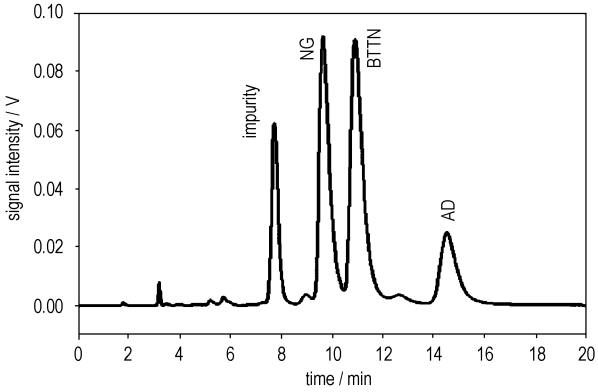
Sensitivity Performances of Several Typical Solid Propellants



NEPE propellant, granule-cast CMDB propellant and screw-extruded CMDB propellant were carried on deflagration-to-detonation transition (DDT) test, detonator sensitivity test and shock sensitivity test respectively, and studied the hazard classification of the three typical solid propellants.

QIN Neng, LIAO Lin-quan, FAN Hong-jie, LI Jun-qiang
Chinese Journal of Energetic Materials, **2010**, **18**(**3**): **324 -329**

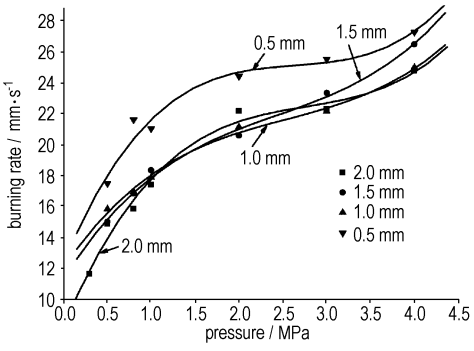
Quantitative Analysis of Migrating Components in Interface of NEPE Propellant/Liner/Insulation



The main migrating components in the interfaces of standard Φ25 mm cylinder samples of nitrate ester plasticized polyether (NEPE) based propellant/hydroxyl terminated polybutadiene (HTPB) based liner/ethylene-propylene-diene terpolymer (EPDM) based insulation were quantified by using high performance liquid chromatography (HPLC) and gas chromatography (GC).

HUANG Zhi-ping, TAN Li-min, CAO Qing-wei, MA Xin-gang
Chinese Journal of Energetic Materials, **2010**, **18**(**3**): **330 -334**

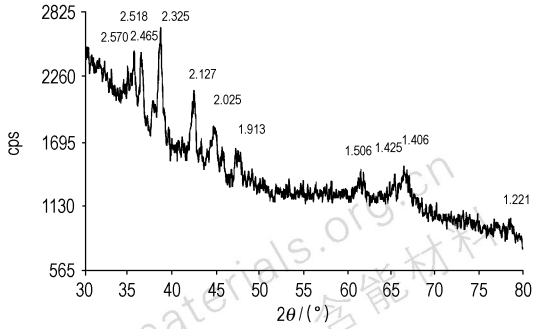
Combustion Characteristics of B/KNO_3 in Microscale Tube



Relation of burning rate of B/KNO_3 and combustor pressure for several different diameter combustors were obtained by experiment. The effect of combustor pressure and combustors diameter on burning rate of B/KNO_3 in microscale tube were analyzed.

LIU Jian, SHEN Rui-qi, YE Ying-hua, HU Yan
Chinese Journal of Energetic Materials, **2010**, **18**(**3**): **335 -338**

Preparation and Characterization of Al-CuO Reactive Bridge Film

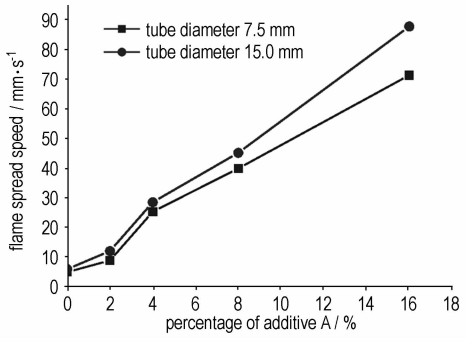


The Al-CuO composite bridge film was ignited using a constant voltage power supply. The phase constitution of the composite bridge film after ignition was investigated by XRD.

HU Yan, YE Ying-hua, SHEN Rui-qi, DONG Neng-fa

Chinese Journal of Energetic Materials,**2010**,**18**(**3**): **339 –342**

Sensitized Performances of Micropore Ball Propellants

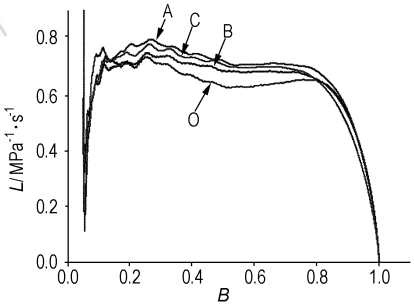


The flame spread speed increases with different sensitizing agents in atmospheric pressure at the loaded condition. With the content of sensitizing agents A increasing, the flame spread speed of the micropore ball propellant increase evidently, and the highest flame spread speed is more than 80 mm · s $^{-1}$.

LIU Yu-jun, LIN Xiang-yang, ZHENG Wen-fang, PAN Ren-ming, LI Sheng-you

Chinese Journal of Energetic Materials,**2010**,**18**(**3**): **343 –347**

Effect of Surface Treatment on Burning Performance of Single-base Gun Propellant

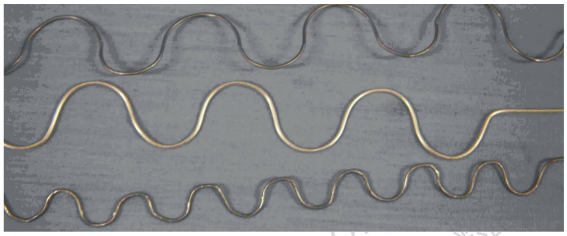


Comparing to original propellant, the activity L of single-base propellant being surface-treated by multibenzylalkyl multiisocyanate has been depressed at ignition stage, and changed more evenly at latter stage. It shows that burning performance of propellant changes obviously, and its changing amounts depend on the surface-treating degree of propellant.

DU Ping, LIAO Xin, WANG Ze-shan

Chinese Journal of Energetic Materials,**2010**,**18**(**3**): **348 –350**

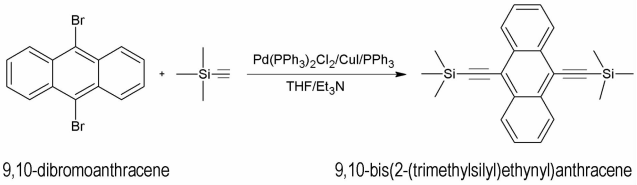
Testing Methods and Factors Affecting Detonation Performance of Mild Detonating Cords



By studying the key affecting factors detonation velocity and shock-wave pressure, primary rules and semi-empirical formula of velocity and shockwave pressure changing were gained. The rules can be used in production process to improve the quality of the detonation cords, and the mild explosive circuit can be designed more accurately.

BAI Ying-wei, WANG Ke-xuan , REN Xi,
AO Cheng-gang, LI Jun, CHU En-yi
Chinese Journal of Energetic Materials,**2010**,**18**(**3**): **351 -355**

Synthesis of Fluorescent Sensors Skeleton 9,10-Bis(trimethylsilylethynyl) Anthracene and Its Spectral Properties

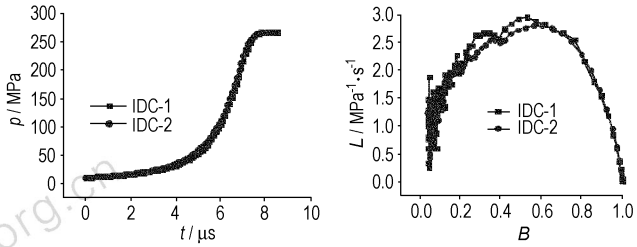


9,10-dibromoanthracene 9,10-bis(2-(trimethylsilyl)ethynyl)anthracene

9,10-Bis(trimethylsilylethynyl) anthracene was prepared by a coupling reaction of dibromoanthracene dibromobenzene and trimethylsilylethyne, using $PdCl_2(PPh_3)_2$ and CuI as catalysts. A mixed solvent of THF/diethylamide was used as the media of the coupling reaction. The product was obtained with desired yields and it was characterized by IR, UV, ^{1}HNMR.

LUO Ya-jun, SHU Yuan-jie, HU Xiao-li
Chinese Journal of Energetic Materials,**2010**,**18**(**3**): **356 -357**

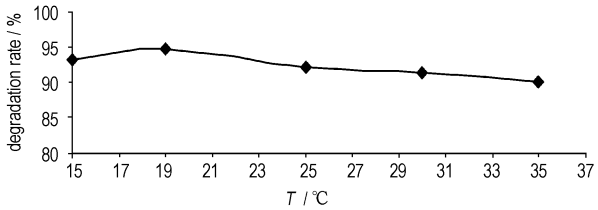
Performance Improvement of Modified Single Base Propellant with a Special Compound



The performance of the propellant were improved significantly through adding a special compound in course of the preparation of the modified single base propellant.

LIU Bo, WANG Qiong-lin, LIU Shao-wu, YU hui-fang,
WEI Lun, LI Da, WANG Feng, ZHANG Yuan-bo
Chinese Journal of Energetic Materials,**2010**,**18**(**3**): **358**

Degradation of UDMH Waste Water by Electrolyzed Oxidizing Water



Degradation of UDMH waste water by electrolyzed oxidizing water was studied.

LIU Yuan, XIA Ben-li, CONG Ji-xin
Chinese Journal of Energetic Materials,**2010**,**18**(**3**): **359 -360**

Executive editor: WANG Yan-xiu Computer typesetter: LI Shao-hui