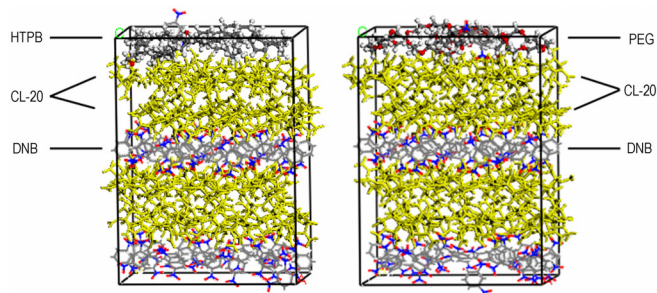


Molecular Dynamics Simulation of Compatibility, Interface Interactions and Mechanical Properties of CL-20/DNB Cocrysal Based PBXs

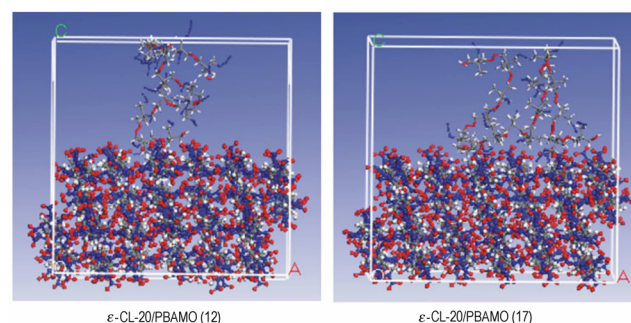
SUN Ting, XIAO Ji-jun, ZHAO Feng, XIAO He-ming
Chinese Journal of Energetic Materials, 2015, 23(4): 309–314



Molecular dynamics simulation (MD) was conducted to investigate the compatibility, interface interactions and mechanical properties of CL-20/DNB cocystal based polymer-bonded explosives (PBXs) using COMPASS force field with NPT ensemble. Two polymers, hydroxyl-terminated polybutadiene (HTPB) and polyethylene glycol (PEG), were respectively put along crystalline surface (0 0 1).

Simulation and Calculation for Binding Energy and Mechanical Properties of ϵ -CL-20/Energetic Polymer Binder Mixed System

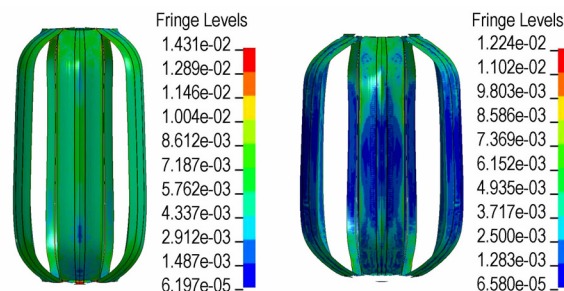
TAO Jun, WANG Xiao-feng, ZHAO Sheng-xiang,
 WANG Cai-ling, DIAO Xiao-qiang, HAN Zhong-xi
Chinese Journal of Energetic Materials, 2015, 23(4): 315–322



To design the formulation of energetic polymer bonded explosives, the energetic binder with different hard and soft segments proportions of AMMO/BAMO was added to the high energy density compound hexanitrohexaazaisowurtzitan (ϵ -CL-20). The binding energy, the interaction modes between the energetic binder and ϵ -CL-20 and the mechanical properties of ϵ -CL-20 / energetic binder systems were simulated by molecular dynamic (MD) method. The enthalpies of formation of the energetic binders with different hard and soft segments proportions were calculated by a group additive method.

Simulation on Initial Velocity and Structure Dynamic Response for Fuel Dispersion

CHEN Ming-sheng, BAI Chun-hua, LI Jian-ping
Chinese Journal of Energetic Materials, 2015, 23(4): 323–329

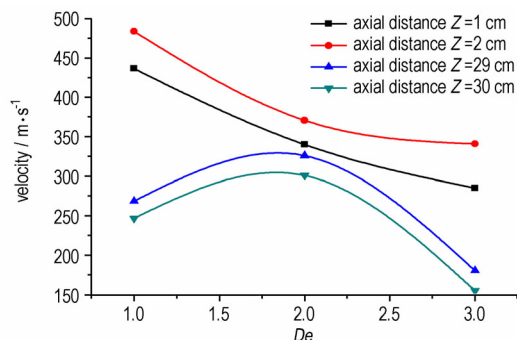


The processes of fuel dispersion and shell breakage driven by central explosive were simulated numerically by LS-DYNA program to study dispersal characteristics for sector cross-section structure. The simulated and experimental results were compared.

Non-ideal Characteristics of Fuel Dispersal Driven by Explosive

SHI Yuan-tong, ZHANG Qi

Chinese Journal of Energetic Materials, 2015, 23(4) : 330–335

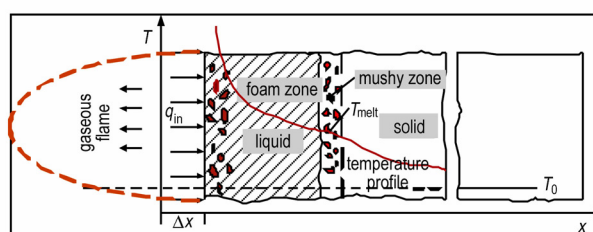


The influence of decouple coefficient (De), the center charge offset and shell weakening in one side on non-ideal characteristics of fuel dispersal were studied by using LS-DYNA.

A Numerical Method of Laser Ignition Characteristic Parameters for HMX Monopropellant

ZHANG Ling-ke, YU Yong-gang, LIU Dong-yao, LU Xin

Chinese Journal of Energetic Materials, 2015, 23(4) : 336–339

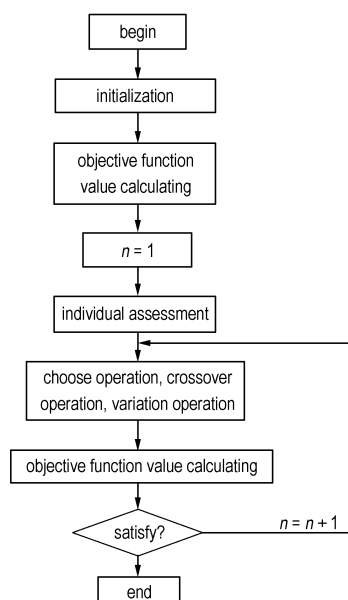


The laser ignition process for solid propellant was divided into three steps, thermal decomposition, boundary layer gas mixing and rapid chemical reaction by deep analysis on the mechanics of laser ignition for solid phase reaction model. The prediction model for ignition delay time and ignition temperature of laser ignition was built.

Application of Genetic Algorithm in Calculation of Combustion Equilibrium Composition

XIE Zhong-yuan, ZHOU Lin, WANG Hao, LI Shou-dian

Chinese Journal of Energetic Materials, 2015, 23(4) : 340–345



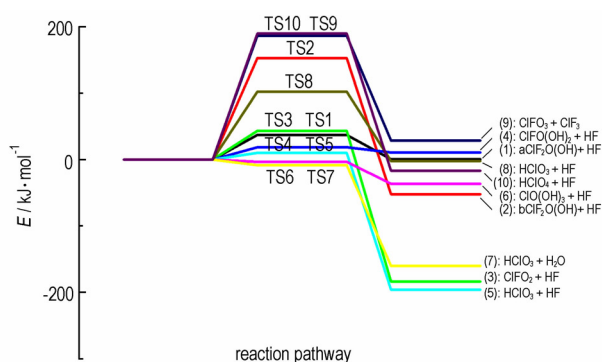
Genetic algorithm for the calculation of combustion equilibrium composition was proposed based on the principles of chemical equilibrium and the method of minimum free energy. By determining the independent variables and its range, the fitness function was confirmed.

Reaction Mechanism of Chlorine Trifluoride Oxide and Water with Density Functional Theory

YAN Hua, LUO Yong-feng, GAO Hong-quan, YAN Peng,

LUO Kun-sheng

Chinese Journal of Energetic Materials, 2015, 23(4) : 346–350



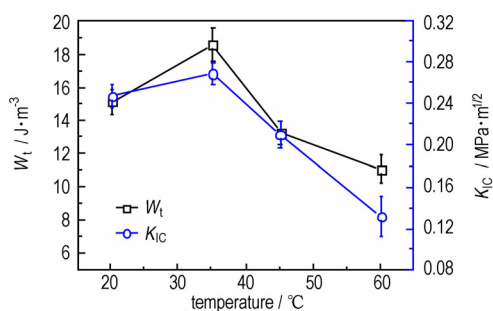
Using density functional theory (DFT), the reaction of chlorine trifluoride oxide with water was studied.

Toughness Measurement of Explosive Based on Fracture Energy of the Stress-strain Curve

WEN Mao-ping, PANG Hai-yan, TANG Ming-feng,

TANG Wei, HE Chuan-lan

Chinese Journal of Energetic Materials, 2015, 23(4) : 351–355

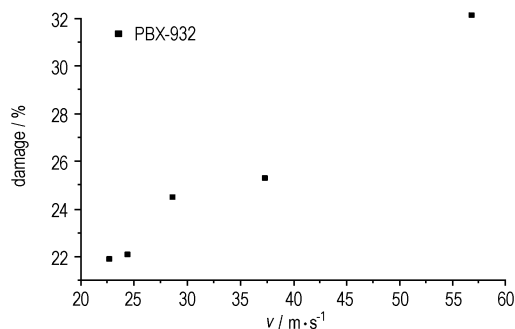


In order to solve the the limits of impact toughness A_k in characterization of explosive fracture toughness, the tensile fracture energy W_t and the compress fracture energy W_c based on the stress-strain curve were put forward. The similarity of the physical meanings between the fracture energy parameters (W_t , W_c) and the impact toughness A_k , was found via analyzing the test principle. W_t , W_c and K_{Ic} for different explosives HMX-P1, HMX-P2, TATB-P3 at room temperature were studied by experiments as well as for HMX-P2 at 20, 35, 45 °C and 60 °C.

Response Characteristics of Polymer Bonded Explosive in Compression and Shear Test

DAI Xiao-gan, WANG Juan, HUANG Qian, SHEN Chun-ying, HUANG Feng-lei

Chinese Journal of Energetic Materials, 2015, 23(4) : 356–361

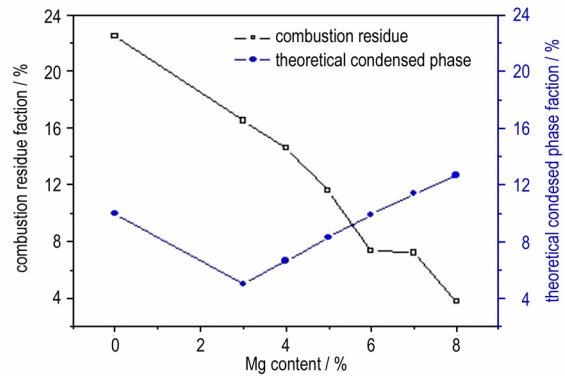


A compression and shear test device was designed. The tests were carried out for polymer bonded explosive. Reaction response was analyzed by measured pressure process, compression deformation and damage characterization.

Influence of Magnesium on Combustion Performance and Artificial Fog Forming Performance of Fog Aerosol

DAI Meng-yan, LIU Xiang-cui, MIN Ping-ting,
FANG Guo-feng, LIU Jiang-hai, CHEN Chun-sheng,
ZHANG Tong

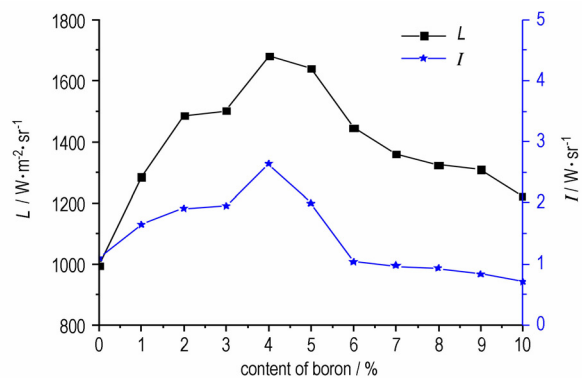
Chinese Journal of Energetic Materials, 2015, 23(4) : 362–367



The combustion temperature, linear burning velocity and combustion residue of fog aerosol were tested. Combined with the calculation results of combustion products and correlative thermodynamic properties of fog aerosol by CEA (Chemical Equilibrium and Application), the influence of Mg on combustion reaction, nucleation process of artificial nucleus and visibility light shielding performance of artificial fog were researched.

Effect of Boron Power on Combustion and Infrared Radiation Characteristics of $\text{KNO}_3/\text{Mg-Al}$ Decoy

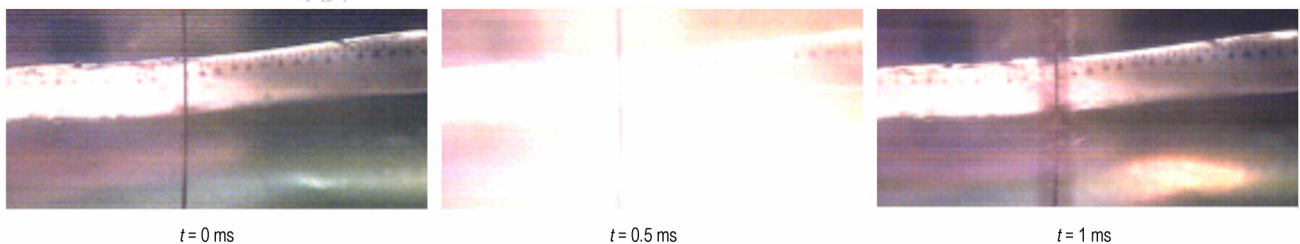
DU Jun, GUAN Hua, LI Jie, GAO Yong, YAO Wen-jia
Chinese Journal of Energetic Materials, 2015, 23(4) : 368–371



To improve the infrared radiation intensity of $\text{KNO}_3/\text{Mg-Al}$ decoy, the combustion and infrared radiation characteristics of the decoy were experimentally studied via the method of adding boron powder in the decoy by a far infrared thermal imager.

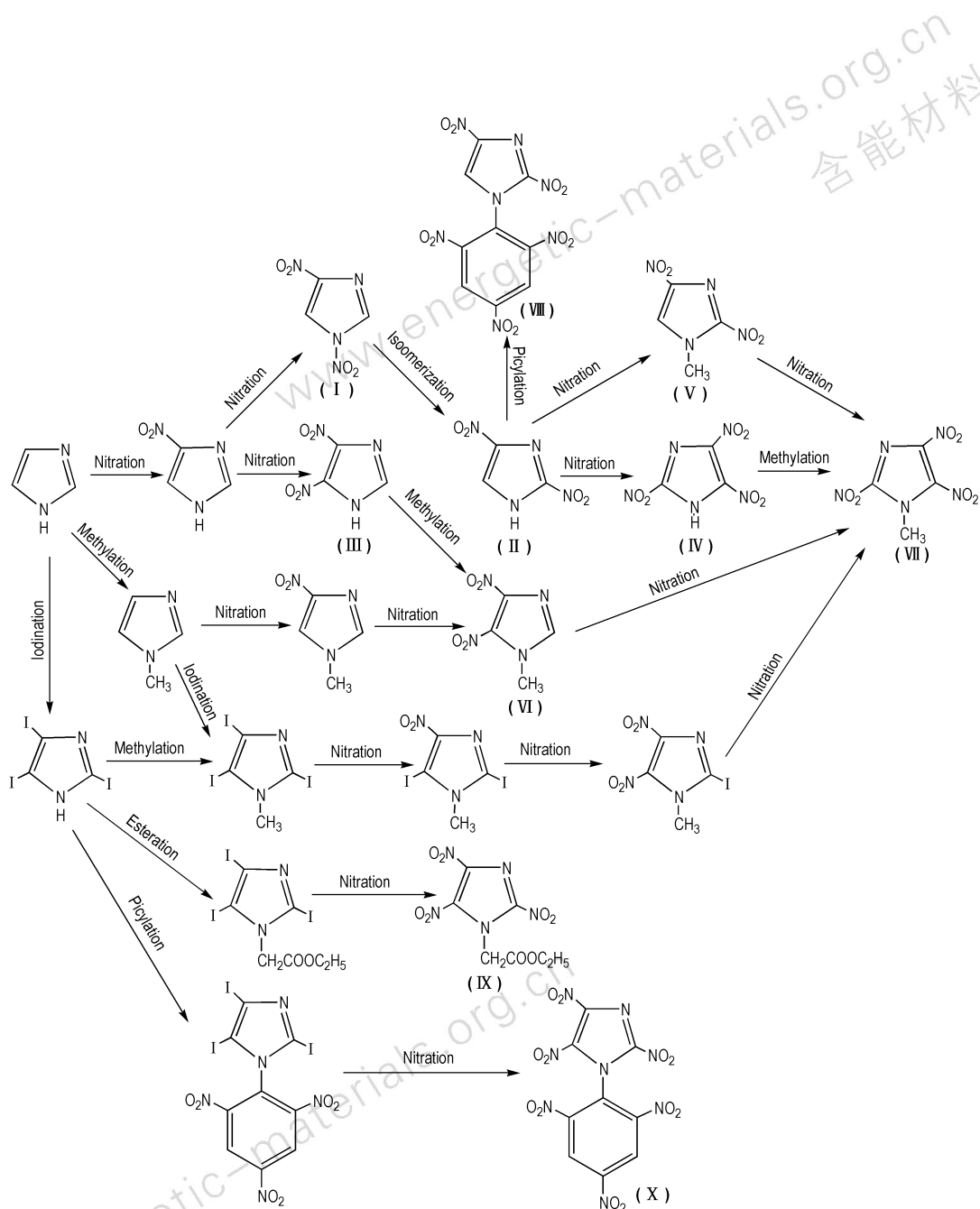
Underwater Explosion Bubble Pulsation Characteristics of Low Energy Detonating Cord

LIN Jia-jian, JIA HU
Chinese Journal of Energetic Materials, 2015, 23(4) : 372–375



An underwater explosion experiment low energy detonating cord was carried out by high-speed photography technology.

Review on Synthesis of Nitroimidazoles Energetic Materials

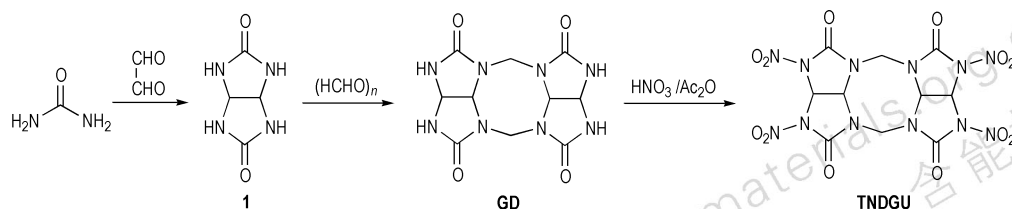


FENG Lu-lu,^{*} CAO Duan-lin, WANG Jian-long, LIU Pei-hong, ZHANG Nan

Chinese Journal of Energetic Materials, 2015, 23(4) : 376–385

The synthetic routes of nitroimidazoles energetic materials and their properties were summarized and described the disadvantages of these schemes, such as 1,4-DNI, 2,4-DNI and MTNI. Hope for to give a assistance for the development of explosives in energetic field.

Progress in Synthesis and Performance of Nitrourea Energetic Materials

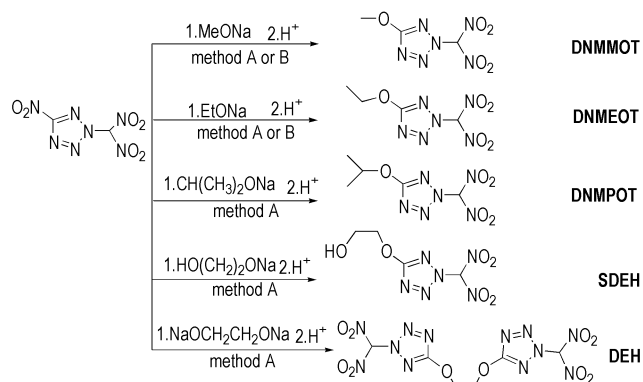


WANG Rui, XU Zhi-bin, MENG Zi-hui, CUI Ke-jian,
LIU Wen-jin

Chinese Journal of Energetic Materials, 2015, 23(4) : 386–400

The synthesis and performance of nitrourea energetic materials were systematically reviewed, and five-membered ring nitroureas, especially glycoluril derivatives, were introduced.

Synthesis of 2-Dinitromethyl-5-alkoxytetrazole

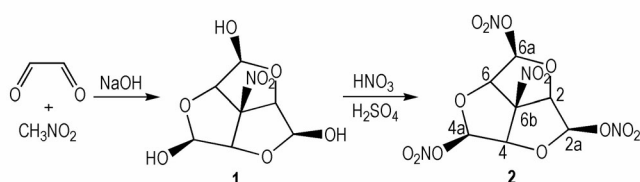


ZHANG Min, BI Fu-qiang, XU Cheng, GE Zhong-xue,
LIU Qing, WANG Wei, WANG Bo-zhou

Chinese Journal of Energetic Materials, 2015, 23(4) : 401–404

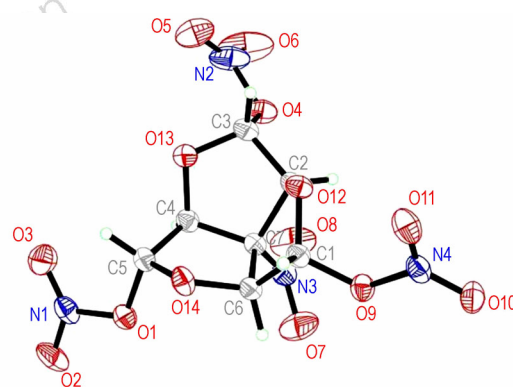
Five novel compounds were synthesized and characterized by IR, NMR, elemental analysis and HPLC-MS. Their detonation performances were predicted by B3LYB method.

Synthesis and Crystal Structure of 6b-Nitrohexahydro-2H-1,3,5-trioxacyclopenta[cd]-pentalene-2,4,6-triyl trinitrate



LI Xiang-zhi, LI Ya-nan, ZHOU Cheng, LI Hui, FAN Xue-zhong,
WANG Bo-zhou

Chinese Journal of Energetic Materials, 2015, 23(4) : 405–408



An energetic plasticizer 6b-nitrohexahydro-2H-1,3,5-trioxacyclopenta[cd]-pentalene-2,4,6-triyl trinitrate was synthesized from glyoxal and nitromethane via the condensation and nitration reaction and its single crystal was studied.

Executive editor: WANG Yan-xiu JIANG Mei ZHANG Qi