Graphical Abstract

Synthesis, Measurement and Correlation of Solubility of Dihydroxylammonium and Alkali Metal Salts of 5,5'-Bistetrazole-1,1'-diolate

5.0 ■ HATO 4.5 Li<sub>2</sub>DHBT 4.0 K<sub>2</sub>DHBT Na<sub>2</sub>DHBT 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 40 45 50 60 35 55 65

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

Chinese Journal of Energetic Materials, 2015, 23(3): 208-212

Dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate, dilithium 5,5'-bistetrazole-1,1'-diolate, disodium 5,5'-bistetrazole-1,1'-diolate and dipotassium 5,5'-bistetrazole-1,1'-diolate were synthesized. Their solubilities were measured and analyzed.

## Synthesis and Properties of 1-Amino-3-nitroguanidinium 4-nitroamino-1, 2, 4-triazole Salt

$$\begin{pmatrix} \mathsf{NH}_2 & \mathsf{O}_2\mathsf{N} & \mathsf{NH} & \mathsf{O}_2\mathsf{N} & \overset{\bullet}{\otimes} \\ \mathsf{N} & \mathsf{Con.H}_2\mathsf{SO}_4 & \overset{\bullet}{\mathsf{N}} & \mathsf{AgNO}_3 & \overset{\bullet}{\mathsf{N}} & \overset{\bullet}{\mathsf{Ag}} \\ \mathsf{N} & \mathsf{N} & \mathsf{HNO}_3 & \mathsf{N} & \mathsf{N} & \mathsf{Ag} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{Ag} \\ \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} & \mathsf{N} \\ \mathsf{N} \\ \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N} \\ \mathsf{N} & \mathsf{N}$$

JIN Xing-hui, HU Bing-cheng, LIU Zu-liang, LV Chun-xu Chinese Journal of Energetic Materials, 2015, 23(3): 213–217 A novel energetic salt 1-amino-3-nitroguanidinium 4-nitroamino-1, 2, 4-triazole salt was synthesized and characterized.

#### Green Synthesis of 2-Nitratomethyltetrahydrofuran

$$\begin{array}{c|c} \text{OH} & N_2O_5 \\ \hline \text{CH}_2\text{CI}_2 \\ \end{array} \begin{array}{c} \text{ONO}_2 \\ \end{array}$$

LIU Ya-jing, MO Hong-chang, LU Xian-ming, LI Lei, GE Zhong-xue

Chinese Journal of Energetic Materials, 2015, 23(3): 218-221

2-nitratomethyltetrahydrofuran ( NMTHF ) was synthesized with 2-hydroxymethyltetrahydrofuran ( HMTHF ) as starting material and dinitrogen pentoxide as nitrating agent. The structure of NMTHF was characterized by IR ,¹H NMR and element analysis, and the optimum nitration conditions was obtained.

# Optimization on Synthesis Process and Characterization of 1-Methyl-3, 4-dinitropyrazoles

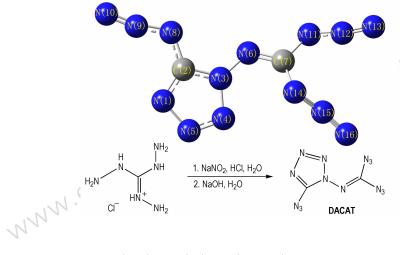
ZHANG Qiao-ling, LI Ya-jin, JIAO Qing-jie, REN Hui, LI Yong-xiang

Chinese Journal of Energetic Materials ,2015 ,23(3): 222-225

1-Methyl-3,4-dinitropyrazole (MDNP) was synthesized using 3-nitropyrazole as starting material via nitration and methylation, and it was characterized by infrared spectrum (IR), proton nuclear magnetic resonance (<sup>1</sup>H NMR) and differential scanning calorimetry (DSC).

□ Graphical Abstract

### Synthesis and Theoretical Study of 1-Diazidecarbonimidoyl-5-azidotetrazole

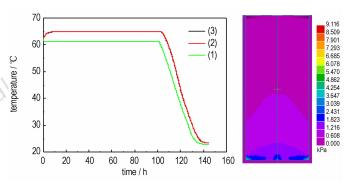


1-Diazidecarbonimidoyl-5-azidotetrazole (DACAT) was prepared via diazotized substitution reaction and cyclization reaction using triaminoguanidinium as raw material. Its structure was confirmed by IR, <sup>13</sup>C NMR and <sup>14</sup>N NMR. The influence of triaminoguanidinium / sodium nitrite molar ratio, reaction temperature, reaction time and pH of system on the yield of reaction was examined. The geometry of DACAT were optimized at the B3LYP/6-31G(d,p) basis set level using a density functional theory(DFT). Theoretical density, enthalpy of formation of gas phase, enthalpy of formation of solid phase, detonation velocity and detonation pressure for DACAT were calculated by Monte-Carlo method, complete base set method (CBS - 4 M) and Kamlet-Jacobs formula, respectively.

XIAO Xiao, LIU Qing, BI Fu-qiang, SU Hai-peng, DING Ke-wei, LI Tao-qi, GE Zhong-xue

Chinese Journal of Energetic Materials ,2015 ,23(3): 226-231

## Experiment and Numerical Simulation Curing Process of Cast PBX



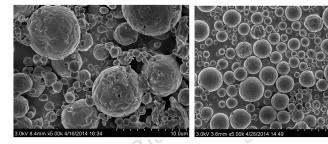
ZHANG Bai-lei, CHANG Shuang-jun, YUAN Jun-ming, OU Ya-peng

Chinese Journal of Energetic Materials, 2015, 23(3): 232-237

To research the change rule of temperature field and stress field in the curing process for cast PBX (Polymer Bonded Explosive, PBX), the temperature field in the curing process of cast PBX under 60  $^{\circ}$ C was tested by Bragg gratings. The numerical simulation of temperature fields and stress fields under different heat transfer coefficient during curing process of the cast PBX explosive were conducted by finite element method.

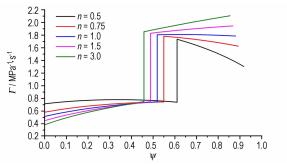
 ${\rm I\hspace{-.1em}I\hspace{-.1em}I}$ Graphical Abstract

Effect of Solvent on the Morphology and Properties of RDX Prepared by the Spray Drying Method



WANG Jiang, LI Xiao-dong, WANG Jing-yu, AN Chong-wei Chinese Journal of Energetic Materials, 2015, 23(3): 238-242 The morphology of spherical RDX which was prepared by spray drying method was analyzed by SEM.

Numerical Calculation of Combustion Property for Seven-hole Variable Burning Rate Gun Propellant



A combustion model of seven-hole variable burning rate gun propellant was established. The function relation of combustion gas generation brisance(  $\Gamma$  ) against the percentage of gun propellant burned (  $\Psi$  ) was deduced. The  $\Gamma$ - $\Psi$  curves were obtained by programming and calculation. The effects of burning rate ratio, inner pore diameter of the fast burning layer, length-to-diameter ratio and thickness of the slow burning layer on the combustion progressive property of seven-hole variable burning rate gun propellant were analyzed.

LIU Ping, MA Zhong-liang, WANG Shuai-yu, CHAI Jun Chinese Journal of Energetic Materials, 2015, 23(3): 243-247

**Experimental Investigation of Boron Combustion in Flow** Field Conditions in Secondary Chamber of Ducted www.energetic-materials. Rocket



Boron based ducted rocket experimental system for ground simulation was established to study the boron combustion. Through heating the boron in a primary chamber by the combustion gas of the ethanol and oxygen, and using air react with boron in the secondary chamber, the working process under the condition of the flow field was simulated, and the similar condition for the real ducted rocket was obtained.

LIU Dao-ping, XIA Zhi-xun, HU Jian-xin, HUANG Li-ya

Chinese Journal of Energetic Materials ,2015 ,23(3): 248-252

IV Graphical Abstract

## Scatter of Projectile Affected by Initial Temperature of AP/HTPB Composite Base Bleed Propellant

ZHANG Ling-ke, YU Yong-gang, LIU Dong-yao, LU Xin *Chinese Journal of Energetic Materials*, 2015, 23(3): 253–257

The initial temperature sensitivity factor ( $\sigma_p$ ) of burning rate for for AP particle was introducue and calculated by three models, Click, Kubota and BDP. Based on the calculated, the inter ballistic model and 6D external ballistic model for a 155 mm base bleed projectile were built and solved simultaneously to simulate the hitting points of the projectile scatter.

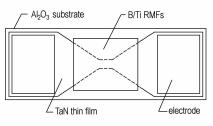
# Effect of Explosive/Tungsten Powder Mass Ratio for LCD Ammunition on Dispersal Characteristics of Tungsten Powder

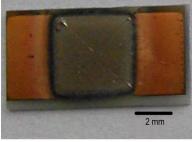
LIU Jun, YAO Wen-jin, ZHENG Yu, LI Wen-bin, WANG Xiao-ming

Chinese Journal of Energetic Materials, 2015, 23(3): 258-264

The effect of charge mass ratio of new low collateral damage ammunition on dispersal velocity of tungsten powder was investigated numerically, theoretically and experimentally.

## Fabrication and Performances of $(B/Ti)_n/TaN$ Thin-film Initiator Bridge





CAI Xian-yao, JIANG Hong-chuan, YAN Yi-chao, ZHANG Yu-xin, DENG Xin-wu, ZHANG Wan-li

Chinese Journal of Energetic Materials, 2015, 23(3): 265-269

(B/Ti)  $_n/TaN$  thin-film initiator bridgewas fabricated by magnetron sputtering and micro-manufacturing technology with the TaN thin-film initiator bridge(80  $\mu$ m×40  $\mu$ m×2  $\mu$ m) and B/Ti multi-layers (4 mm ×4 mm). The ignition performances of the (B/Ti)  $_n/TaN$  thin-film initiator bridge and TaN thin-film initiator bridge were tested by a 47  $\mu$ F tantalum capacitor with voltage of 40 V.

### Reliability Analysis for Explosive Initiator Based on Generalized Linear Models

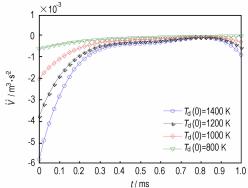
HONG Dong-pao, WANG Ying-hua, GUAN Fei, WEN Yu-quan

Chinese Journal of Energetic Materials, 2015, 23(3): 270-274

A method based on generalized linear models of reliability analysis for explosive initiator was proposed according to sensitivity test and characteristics of reliability analysis. The likelihood function was transformed to be a generalized linear expression of binomial variable. Using the generalized linear model for binomial distribution, the maximum likelihood estimations of the model coefficients were obtained, and corresponding arithmetic was put forward.

V Graphical Abstract

Effects of Particles Characteristics at High-temperature on Bubble Dynamic Behaviors and Acoustic Radiation Characteristics

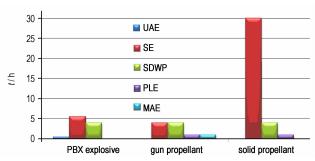


Bubble dynamic model was deduced based on the heat transfer and mass transfer theory to investigate the characteristic of the acoustic radiation induced by the interaction between water and high temperature particles produced by underwater combustion of pyrotechnic composition. The effect of initial temperature and radius for high temperature particles on the bubble dynamic behaviors and acoustic radiation characteristics were calculated and analyzed.

OUYANG Di-hua, KOU Wei-cai, DUAN Dong-li

Chinese Journal of Energetic Materials, 2015, 23(3): 275-278

Sample Pretreatment Techniques for the Chromatographic Analysis of Energetic Materials



The extraction effect of PBX, gun propellant and solid propellant by the ultrasound-assisted extraction (UAE), microwave-assisted extraction (MAE), pressurized-liquid extraction (PLE), Soxhlet's extraction (SE) and solventdissolve-water-precipitation extraction (SDWP) were examined.

JIA Lin, ZHANG Gao, ZHANG Lin-jun, ZHANG Dong-mei, DU Jiao-jiao, WANG Qiong, YANG Cai-ning, REN Chun-yan Chinese Journal of Energetic Materials ,2015 ,23(3): 279-284

Mass Transfer-Reaction Process of NO Gas Absorbed by www.energetic-material Fe II (EDTA) 2- Solution

25 experiment value calculated value 20  $N_A \times 10^5 / \text{ mol·m}^2 \cdot \text{s}^{-1}$ 15 10 200 400 800 1000 1200 1400  $C_A / \text{mg} \cdot \text{m}^{-3}$ 

A ferrous complex Fe II (EDTA) 2- was used as the absorbent of NO in a bubbling reactor. The effects of absorbing solution concentration and NO gas concentration on the absorption rate were studied. The mass transfer reaction process of NO absorption was analyzed. A theoretical model describing the NO absorption process was derived.

WANG Fei, LIU You-zhi, YUAN Zhi-guo, QI Gui-sheng,

Chinese Journal of Energetic Materials, 2015, 23(3): 285-290

VI Graphical Abstract

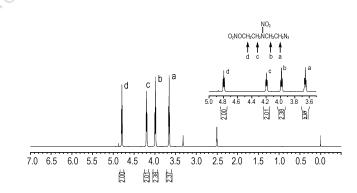
### Review on Bis-azoles and its Energetic Ion Derivatives

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

Chinese Journal of Energetic Materials, 2015, 23(3): 291-301

The progresses and properties of bis-1,2,4-triazoles, bistetrazoles, 5-(1,2,4-triazol-3-yl) tetrazoles and its energetic ion derivatives were reviewed. Nine kinds new type bis-azoles were designed and their performance were predicted by quantum chemistry methods. Researches on the law of various nitrogen-rich cations on sensitivity and detonation performance of bis-azoles and synthesis of new type bis-azoles with better performance are the keys of further work.

Synthesis and Characterization of Pentanol-3-nitraza-5-azidonitrate



GAO Fu-lei, JI Yue-ping, LIU Wei-xiao, WANG Ying-lei, CHEN Bin, LIU Ya-jing, DING Feng

Chinese Journal of Energetic Materials, 2015, 23(3): 302-303

Pentanol-3-nitraza-5-azidonitrate (PNAN) (crude product) was designed and synthesized for the first time via reaction in dimethyl sulfoxide, using 1, 5-dinitrato-3-nitraza pentane (DINA) and sodium azide as raw materials The crude product was separated and purified bysilica gel column chromatography. The structure of the purified product was characterized by IR, <sup>1</sup>H NMR and elemental analyses. Some physicochemical properties of PNAN were also studied.

## One-step Synthesis and Thermal Behavior of 1-Methyl-3,4,5-trinitropyrazole

GUO Jun-ling, LI Yong-xiang, WANG Jian-long, CAO Duan-lin, WANG Yan-hong, WANG Shao-lin

Chinese Journal of Energetic Materials ,2015 ,23(3): 304-306

1-Methyl-3,4,5-trinitropyrazole (MTNP) as an insensitive energetic compound was one-step synthesised by direct nitration of 1-methylpyrazole in nitric acid and fuming sulfuric acid for the first time.

Executive editor: WANG Yan-xiu JIANG Mei ZHANG Qi