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花开并蒂  
Blooming side by side

三唑类含能化合物研究进展  
Review on Energetic Compounds Based on Triazoles

HANNENG CAILIAO

2023  
第31卷 5



现代战争对武器弹药与能源系统要求(高能量密度、低特征信号和环境友好等)逐步提高,唑类含能化合物因为具有高标准生成焓、高密度、低感度和产物为氮气等诸多优点,成为国内外研究热点。富氮杂环骨架中,基于三唑环兼顾高热稳定性和高正生成焓的特点,成为构筑高能量密度材料(HEDMs)的有效结构单元。此外,通过在三唑环引入不同的含能基团,可能对三唑类含能材料进行有效的结构设计 with 性能调控,在极大丰富三唑环含能化合物种类的同时,也满足了不同的应用需求。来自**中北大学**的**刘洋**、**张树海**等研究人员综述了近些年来国内外关于五种(单环三唑类、双环三唑类、吡唑基三唑类、噁二唑基三唑类以及四唑基三唑类)三唑类系列40余种含能化合物的最新研究成果,综述包含了这些化合物的化学结构、合成路线等,并对部分化合物的性能进行了相应的阐述。通过与传统硝胺类炸药RDX和HMX的性能对比发现,三唑类含能化合物的具有高热稳定性、高密度、钝感等特性。期望通过对三唑类含能化合物的合成方法、结构与性能综述,为未来设计和合成综合性能为优异的三唑类含能化合物提供了参考。

花开并蒂

封面以夏日的荷景为背景,代指本综述三唑类含能化合物的研究“热”点。映照的水面指代整体含能材料研究领域,并蒂莲花代表两种典型的含能三唑环,并蒂莲开在静谧的水面暗指三唑类含能化合物隶属于整体含能材料领域的研究之中。并蒂莲上的两种三唑环代表着两者互为同分异构体,为含能材料的发展做出了突出的贡献。水面上其它位置的莲花指代不同三唑环含能化合物的不同结构设计 with 性能关系;莲花的盛开则代表三唑环是构筑高能量密度材料的有效结构单元,从而被广泛研究。整体水墨画的封面设计与三唑类含能材料与并蒂莲的合理联想加之夏日荷景,与综述文章启发性的内容一样,亦极具有观赏性。

封面效果 / @山鹰·翼简设计

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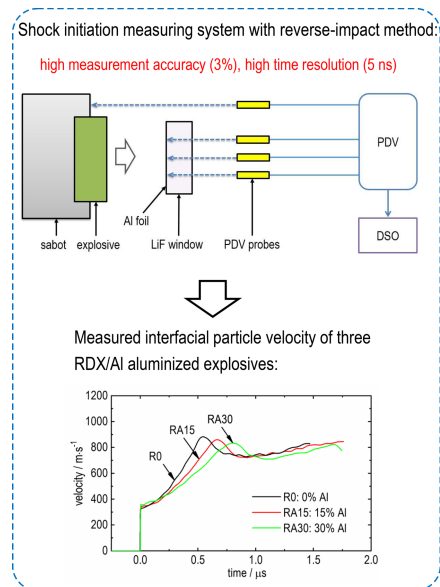
后插 《含能材料》第二届青年学术沙龙暨第三届青年编委会议成功举办

## Explosion and Damage

### Shock Initiation Measurement of RDX-based Aluminized Explosives with Reverse-impact Method

PEI Hong-bo, LI Shu-rui, GUO Wen-can, ZHANG Xu, ZHENG Xian-xu

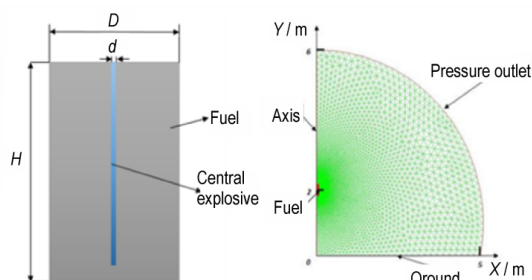
**P425** A shock initiation measuring system was developed based on the reverse-impact method. The explosive sample was driven by a 57 mm gas gun and impacted the LiF window at a certain speed. The photonic doppler velocimetry (PDV) was adopted to measure the interfacial particle velocity profile between the explosive sample and window. Using this measuring system, details of shock initiation of aluminized explosives were measured. Three RDX-based aluminized explosives with different contents of aluminum powder were measured, which are 0, 15% and 30%, respectively, in order to investigate the effect of aluminum on the shock initiation properties of aluminized explosives. The interfacial particle velocity profiles of the three explosives were compared and the mechanism that aluminum powder makes the shock sensitivity decrease was also discussed.



### Numerical Simulation of Cloud Detonation at high Falling Velocity

SU Zhen, GAO Hong-quan, ZHAO Hong-wei, ZHANG Qi

**P431** In this study, the hydrodynamics software Fluent was used to study the dispersion and detonation process of high falling velocity clouds and the fuel dispersion process under high falling velocity conditions, and analyze the shape, radius and concentration distribution of cloud and fog with high falling velocity. The propagation law of temperature and pressure and the peak value of detonation pressure at different distances during cloud detonation were studied. The exploration and establishment of numerical algorithm for high-speed cloud dispersion and detonation process were supplemented.

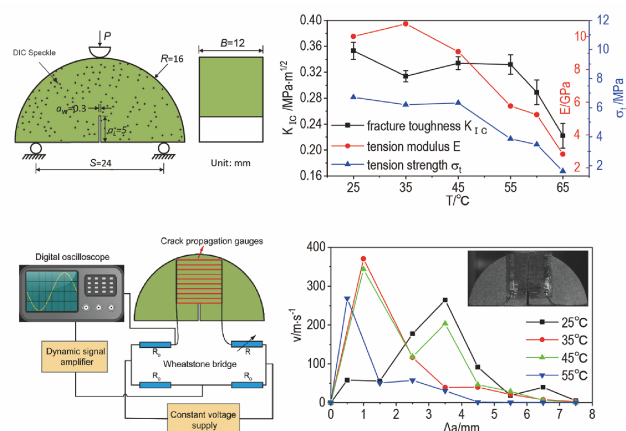


## Safety Performance and Assess

### Temperature Effects on the Fracture Behavior of HMX-Based PBX Under Quasi-Static Loading

DONG Tian-bao, YUAN Hong-wei, WEN Qian-qian, PANG Hai-yan, ZHAO Long, LI Yun-xin

**P440** The fracture behavior of HMX-based PBX at different temperatures were investigated with the digital image correlation method (DICM) and crack propagation gauge (CPG) testing system. The temperature effects on the fracture characteristics, fracture resistance, damage tolerance and crack unstable propagation rate of the HMX-based PBX were studied by using the semi-circular bending (SCB) specimen under quasi-static loading. This study can provide a reference for experimental method for the study of fracture behavior of PBX, and be helpful for understanding of the fracture mechanisms of PBX at different temperatures, as well as provide model parameters and calibration for numerical simulation of PBX fracture.

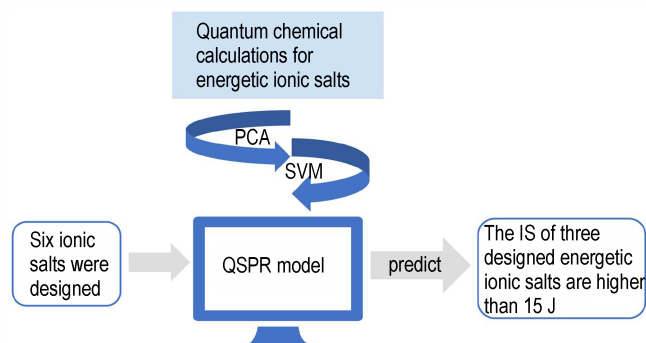




## Application of Support Vector Machine in Quantitative Structure-Property Relationship Study of Impact Sensitivity for Nitrogen-Rich Energetic Ionic Salts

ZHANG Yun-ling, BAI Yang

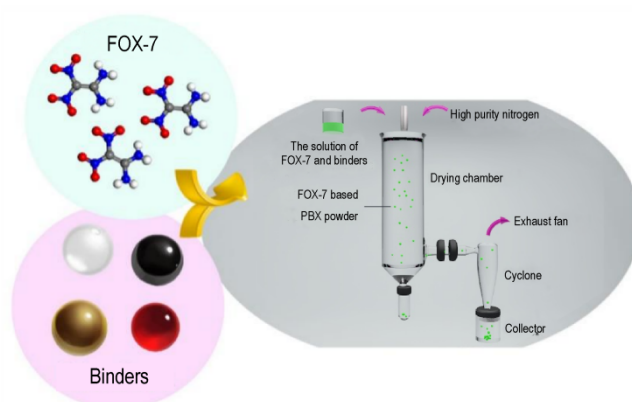
**P448** The quantitative structure-property relationship study (QSPR) between *IS* and molecular structure descriptors ( $E_{\text{HOMO}}$ ,  $E_{\text{LUMO}}$ ,  $\mu$ ,  $\alpha$ ,  $OB$ ,  $NICS$ ,  $\Delta V$ ,  $\sigma^2$ ,  $I$  and  $A$ ) of energetic ionic salts was established for the first time. The QSPR was built by principal component analysis (PCA) combined with support vector machine (SVM). Moreover, six new nitrogen-rich energetic ionic salts were designed and their *IS* were predicted by the built QSPR model. The study provides some reference for the design of new insensitive energetic ionic salts.



## Effect of Binders on Properties of FOX-7 based PBXs by Spray Drying

YANG Yue, LI Xiao-dong, DONG Zi-wen, KONG Song, WANG Jing-yu

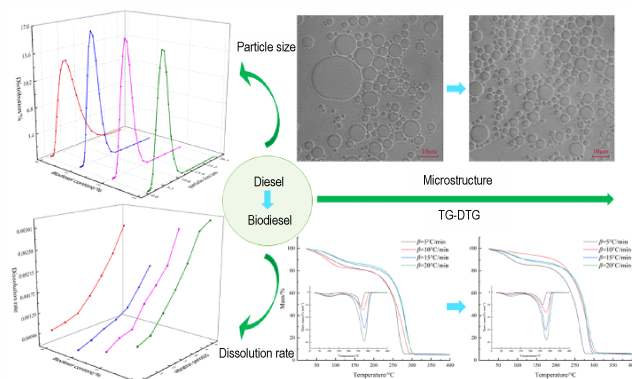
**P457** To get accurate information of the compositing mechanism of polymer bonded explosives (PBXs) prepared by spray drying, FOX-7 based PBXs with different binders were prepared at the presence of Estane 5703,  $F_{2314}$ ,  $F_{2602}$  and ACM, respectively. The effects of binder types and contents on the performance of FOX-7 based PBXs were investigated. The surface morphology, crystalline states, thermal decomposition properties and impact sensitivity of the samples were characterized respectively. The compositing structure and desensitization mechanism of binders in spray-dried PBXs were further analyzed based on the microscopic morphology of FOX-7 based PBXs in molten state. The comparative study of impact sensitivity, atomic ratio of surface elements and chemical state changes of refined FOX-7 and PBXs were carried out to verify them.



## Effect of Biodiesel on Thermal Decomposition Characteristics and Anti-vibration Performance of On-site Mixed Emulsion Explosives

YANG Ce, LI Hong-wei, YANG Sai-qun, SUN Jian-hui, ZHANG Bin-bin

**P467** As a clean energy material, biodiesel has the possibility to be used as the oil phase of on-set mixed emulsion explosive. However, it is not clear whether the use of biodiesel affect the thermal safety and stability of explosives during transport. Under this background, the on-set mixed emulsion explosives with different biodiesel contents were studied by internal phase particle size test, thermal analysis technology and anti vibration experiment.



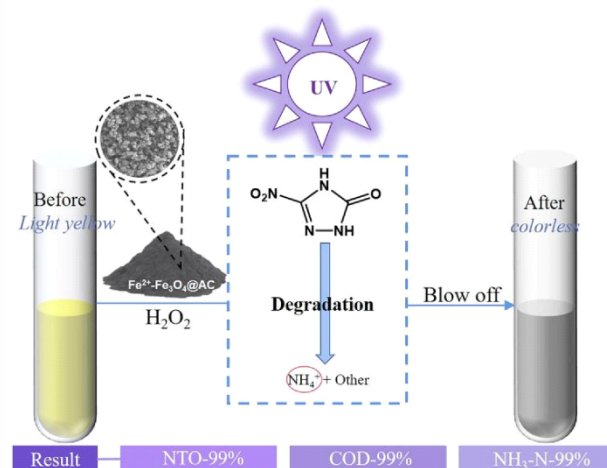


## Environment-friendly Technologies

### Treatment of NTO Washing Water with Heterogeneous Photo-fenton Oxidation-blowing off

GONG Sai-hua, LU Zhi-yan, LI Zhi-hua, CAI Chun

**P477** This study firstly proposed a method for treating NTO washing water in the production with the advantages of being highly efficient, environmentally friendly and no other organic pollutants added. Heterogeneous photo-fenton degrade and then blow off the washing water can remove NTO and reduce COD and  $\text{NH}_3\text{-N}$ . This study included the preparation of catalyst, studying the influence of degradation conditions and speculating on the possible mechanism.

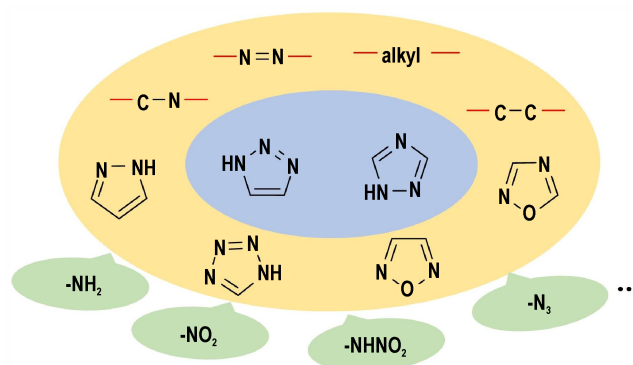


## Reviews

### Review on Energetic Compounds Based on Triazoles

LIU Yang, CHEN Ya-hong, GOU Rui-jun, ZHANG Shu-hai

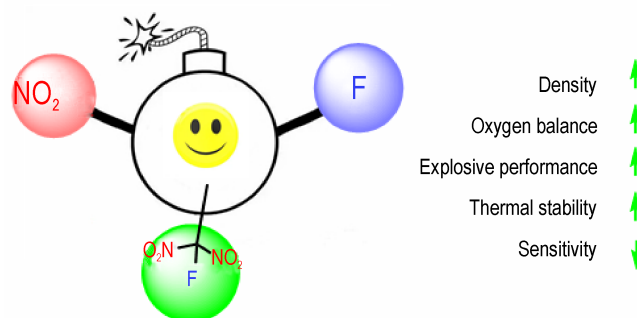
**P485** The research progress of triazole-based energetic compounds was reviewed. The synthetic routes and properties of triazole-based energetic compounds were introduced.



### Progress in the Synthesis and Properties of Fluorodinitromethyl Energetic Compounds

WANG Shao-qing, YIN Hong-quan, MA Qing, CHEN Fu-Xue

**P508** The research of synthesis and properties of fluorodinitromethyl substituted energetic compounds were reviewed.



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