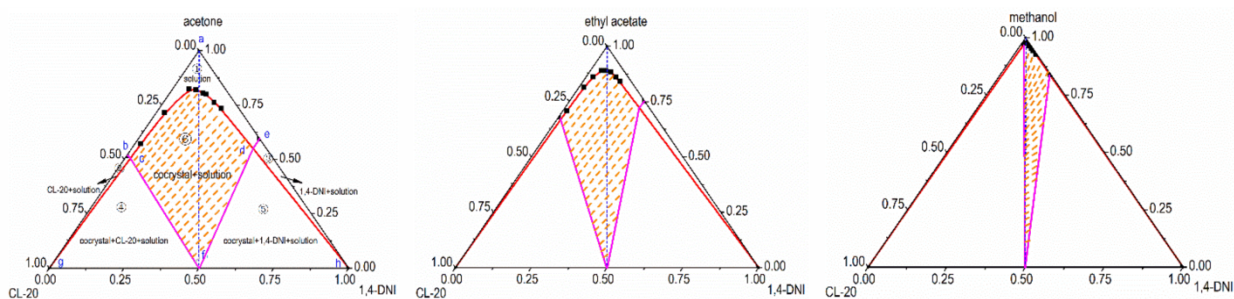


### Thermodynamic on the Formation of CL-20/1,4-DNI Cocystal



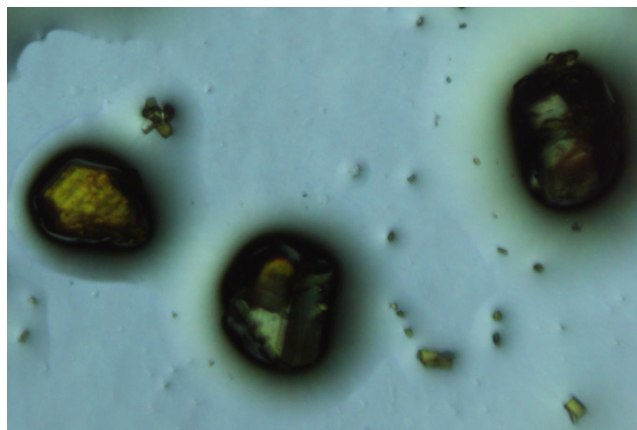
DONG Hai-yan, LONG Yi-qiang, ZHOU Ting-ting, WU Bo,  
DUAN Xiao-hui

*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
2020,28(9):819–825

The thermodynamics of CL-20/1,4-DNI cocrystal formation has been investigated by building the ternary phase diagrams of CL-20/1,4-DNI solvents and calculating the thermodynamic parameters of the solubility product  $K_{sp}$ , the complexation constant  $K_{11}$ , and the reaction free energy  $\Delta G^\ominus$ . The effects of crystallization solvents and temperatures on thermodynamics of CL-20/1,4-DNI cocrystal formation were taken into account.

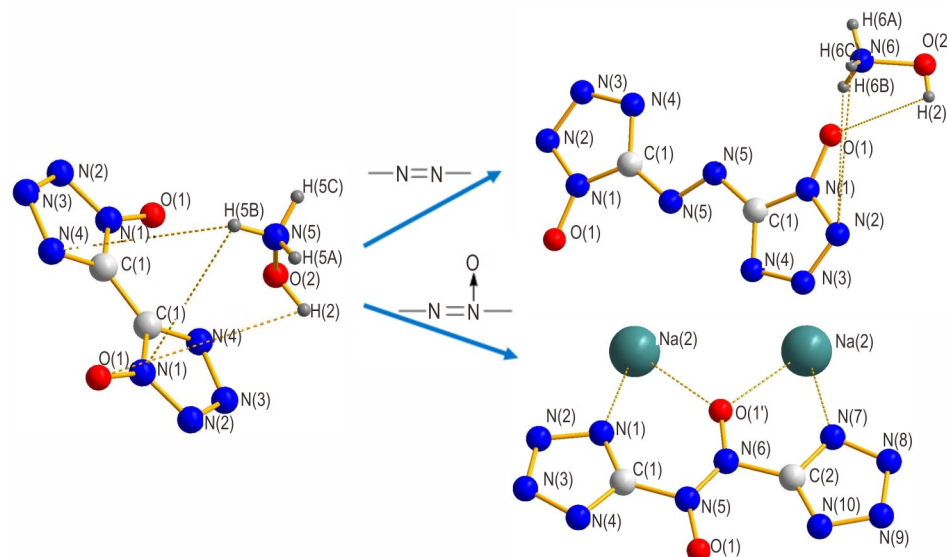
### Crystallization Thermodynamics of FOX-7 in DMSO-EAC Solvent Mixtures

ZHAO Xin-hua, CHEN Li-zhen, WANG Jian-long, HAN Zi-hao  
*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
2020,28(9):826–833



The solubility of FOX-7 in DMSO-EAC mixed solvents were tested. The thermodynamic parameters, solid-liquid surface tension and crystal surface entropy factor of FOX-7 were estimated. The cooling crystallization experiment was carried out in DMSO-EAC mixed solvent.

## Effects of Three Types of Molecular Connection on Crystal Structures and Energetic Properties of Bis-tetrazolium Compounds

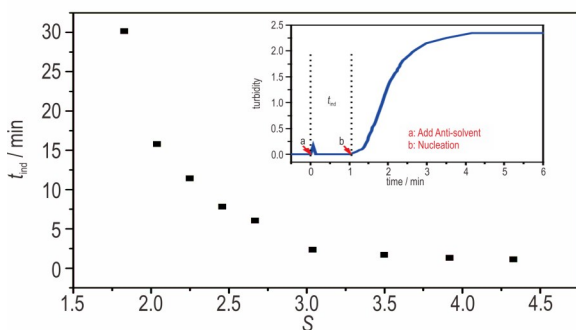


The effects of the introduction of  $\text{—N=N—}$  and  $\text{—N=N(O)—}$  bonds into the structure of bis-tetrazolium compounds were discussed in this work, the crystal structures and properties of three bis-tetrazolium energetic materials, including dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate (TKX-50), dihydroxylammonium azotetrazole-1,1'-diolate (ATZO-1) and sodium 5,5'-azotetrazole-5-oxide pentahydrate (ATO-Na), were compared and analyzed.

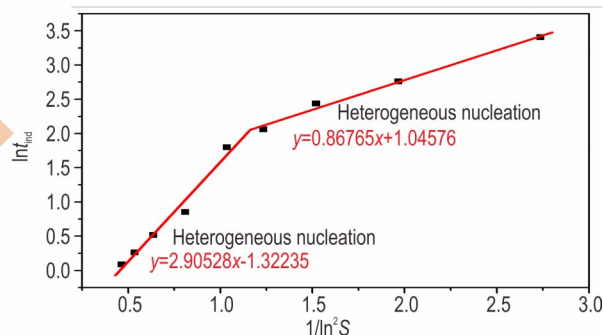
LIN Qiu-han, LI Xin, WANG Peng-cheng, LU Ming

*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
2020,28(9):834–840

## Effect of Supersaturation on Nucleation of LLM-105 Based on Induction Period Measurement Method



classical  
nucleation theory

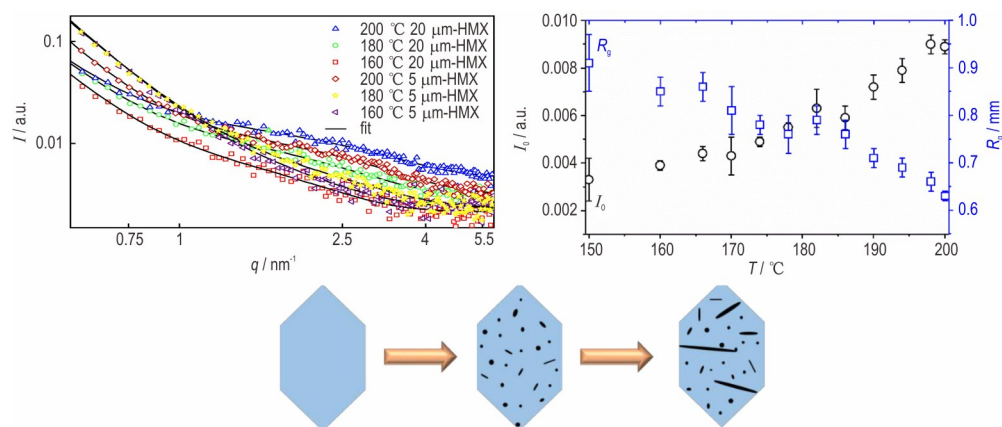


The influence of supersaturation on the nucleation of LLM-105 was investigated based on the induction period measurement method. The nucleation induction periods of LLM-105 with different supersaturation ratios were obtained by measuring the turbidity. Based on the results of anti-solvent crystallization experiments and the classic nucleation theory, the nucleation and growth mechanisms of LLM-105 were determined.

SHAN Jun-hui, ZHOU Xiao-qing, LI Hong-zhen, LIU Tian-sheng

*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
2020,28(9):841–847

### Microstructure of HMX crystallites studied by in situ variable-temperature small-angle X-ray scattering

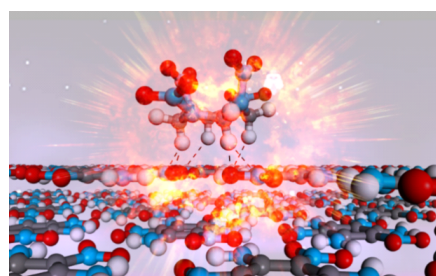


SHI Jing, LIU Jia-hui, BAI Liang-fei, YAN Guan-yun,  
DUAN Xiao-hui, TIAN Qiang

*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
2020,28(9):848–853

The microstructure of HMX (Octogen) crystal particles with average sizes of 5  $\mu\text{m}$  and 20  $\mu\text{m}$  was studied by in situ variable-temperature small-angle X-ray scattering (SAXS) and wide-angle X-ray scattering (WAXS).

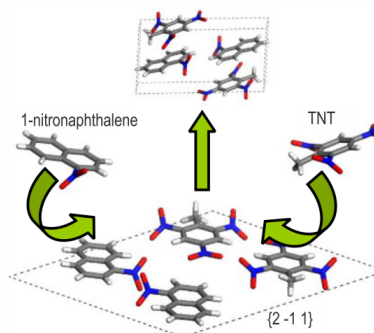
### Theoretical Study on Improvement Strategy of Crystal Stability and Detonation Energy of Cocystal Explosive



LI Chong-yang, HUANG Yong-li, SUN Chang-qing, ZHANG Lei  
*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
2020,28(9):854–860

The effect of hydrogen bonding in regulating crystal stability and detonation energy for 16 reported cocystal explosive crystals.

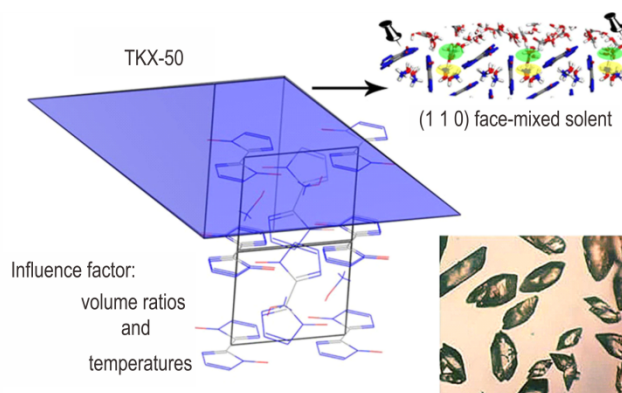
### TNT/NNAP Cocystal Formation Mechanism via Grinding Process



YI Zhen-xin, ZHANG Yu, WANG Tian-ping, ZHANG Lin,  
ZHU Shun-guan  
*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
2020,28(9):861–864

The formation of TNT/NNAP cocystal via grinding process was investigated. Powder XRD illuminated the lattice plane changes while FTIR showed the inter and extra-molecular forces changes. DSC results indicated the phase change of TNT/NNAP cocystal during the process.

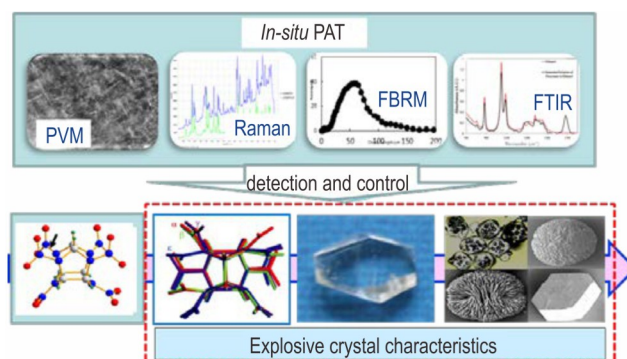
### Growth Morphology of TKX-50 in Formic Acid/Water Mixed Solvent by Molecular Dynamics Simulation



ZHOU Tao, CHEN Fang, LI Jun, CAO Duan-lin, WANG Jian-long  
*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
 2020,28(9):865–873

Crystal morphology predictions of TKX-50 under different formic acid/water volume ratios and temperatures.

### Research Progress and Suggestion for the Modification of the Explosive Crystal Characteristics



LI Hong-zhen  
*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
 2020,28(9):874–888

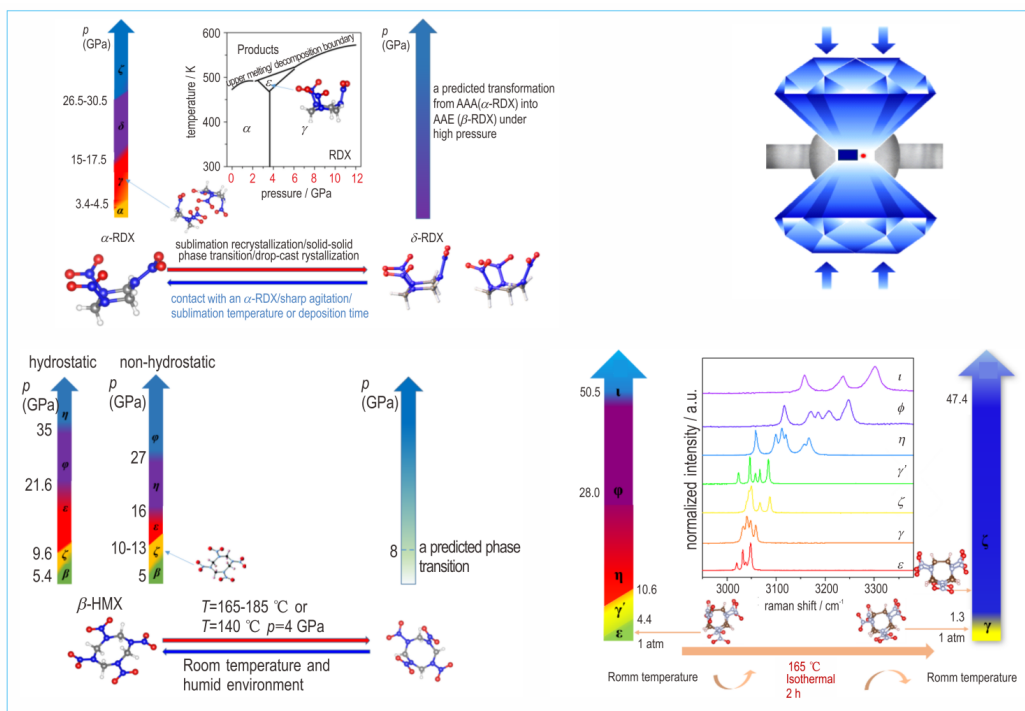
This review summarizes the control principle and process methods of polymorph, crystal quality, particle shape and aggregated structure of explosive crystals and their structure-activity relationship. The challenges and suggestion are also discussed.

### Characteristics and Enlightenment from the Intermolecular Interactions in Energetic Crystals

ZHANG Chao-yang  
*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
 2020,28(9):889–901

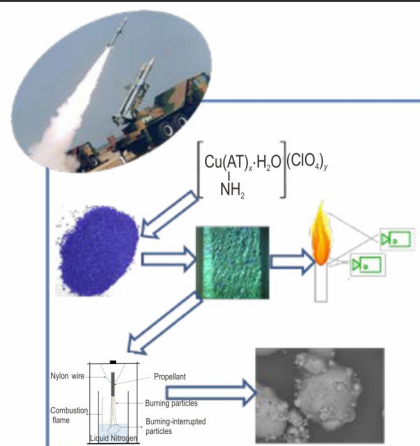
The intermolecular hydrogen bonding, halogen bonding and  $\pi$ - $\pi$  stacking in energetic crystals, and their influences on molecular stacking pattern, impact sensitivity and thermal stability are reviewed.

## Review on Phase Transition of RDX, HMX and CL-20 Crystals under High Temperature and High Pressure



GAO Chan, SUN Xiao-yu, LIANG Wen-tao, LI Xiang-dong,  
 ZHANG Yang, DAI Ru-cheng, WANG Zhong-ping,  
 ZHANG Zeng-ming  
*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
 2020,28(9):902–914

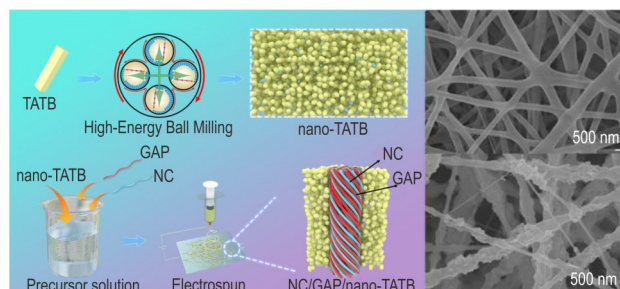
## High Pressure Combustion Characteristics and Atmosphere Pressure Flame Structure of ACP-containing Hydroxyl Terminated Polybutadiene (HTPB) Propellants



MENG Ling-chao, RAN Xiu-lun, LI Jian-min, ZHOU Xu-yuan,  
 GUO Yan-pei, GONG Li, YANG Rong-jie  
*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
 2020,28(9):915–924

In order to investigate the high-pressure combustion characteristics and atmosphere pressure flame structures of HTPB propellant with ACP, three kinds of HTPB propellants with and without ACP were manufactured. High-speed photography system was employed to monitor the combustion process of ACP on the combustion flame structure and the burning surface. The combustion surface and quenched surface were obtained for morphology and composition analysis.

### Characterization and Thermochemical Properties of NC/GAP/nano-TATB Electrospinning Composite Fibers with 3D Network Structure

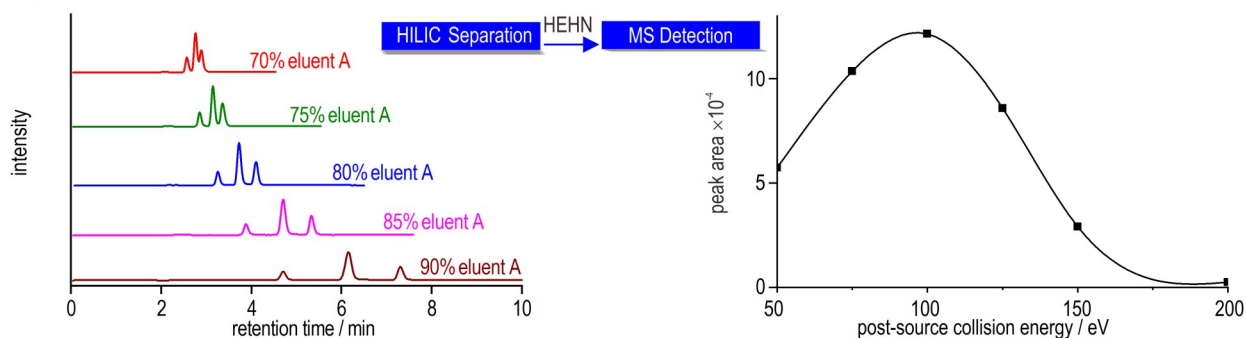


Nanocomposite energetic fibers have been prepared by electrospinning. Its thermochemical properties were investigated and the energy performances were analyzed from the perspective of the formation enthalpy ( $\Delta H_f$ ), oxygen balance (OB), and C/H mass ratio.

LUO Ting-ting, WANG Yi, LIU Li-xia, SONG Xiao-lan

*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
2020,28(9):925–935

### Determination of Hydroxyethyl Hydrazine Nitrate by Hydrophilic Interaction Chromatography Coupled with Mass Spectrometry

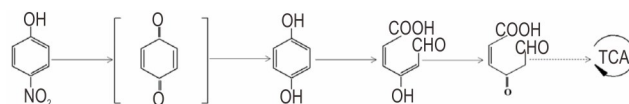


XU Lin-nan, ZHANG Xue-jun, ZHAO Tan, LI Jun, FANG Tao

*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
2020,28(9):936–941

A method of determination of hydroxyethyl hydrazine nitrate (HEHN) by hydrophilic interaction chromatography (HILIC) coupled with mass spectrometry (MS) was developed.

### Effects of Different Factors on PNP Degradation by *Rhodospira sphaeroides* and Metabolic Mechanisms



BAI Hong-juan, SUN Hui-min, ZHANG Qing

*Chinese Journal of Energetic Materials (Hanneng Cailiao)*,  
2020,28(9):942–950

The intermediate products of PNP degradation by *Rhodospira sphaeroides* H strain were detected by HPLC-MS.

Executive editor: GAO Yi JIANG Mei WANG Yan-xiu