Effect of Hydrogen Bonding in Pentazole Nonmetallic Salts



Based on the analysis of hydrogen bond length, strength, number, and N—N bond length in non-metal salts of N_5^- anion, the thermal decomposition temperature is used as the basis for determining the stability. N_5^- anion is easy to form two major types of hydrogen bonds,N—H…N and O—H…N, with electropositive fragments. One of the key factors improving stability is maintaining good structural symmetry after being subjected to hydrogen bonding, the other is forming planar layered graphene-like structures through hydrogen bonding.

WANG Peng-cheng, JIANG Zhen-ming, ZHOU Xin-li, LIN Qiu-han, LU Ming

Chinese Journal of Energetic Materials (Hanneng Cailiao), 2020,28(7):591-596

Generation of Metal-doped Nitrogen Clusters with High Nitrogen Content by Liquid Nitrogen Cooling-laser Ablation



DING Ke-wei, LI Tao-qi, XU Hong-guang, BU Jian-hua, YANG bin, ZHENG Wei-jun, GE Zhong-xue

Chinese Journal of Energetic Materials (Hanneng Cailiao), 2020,28(7):597-602

The conventional laser ablation ion source was improved by adding liquid nitrogen cooling and its effect on generating metal doped nitrogen clusters with high nitrogen content was studied.

CHINESE JOURNAL OF ENERGETIC MATERIALS

Synthesis and Thermal Stability of 4-Azido-2, 2, 6, 6-tetranitroadamantane



CAI Rong-bin, ZHANG Jian, LUO Jun

Chinese Journal of Energetic Materials (Hanneng Cailiao), 2020,28(7):603-608

Synthesis and Properties of a Heat-resistant Biligand Energetic Metal-organic Framework Material A high thermal stable and cage-like energetic compound 4-azido-2,2,6,6-tetranitroadamantane was synthesized from diethyl malonate and paraformaldehyde *via* 8 steps with a total yield of 9.8%.



The double ligand E-MOFs was prepared by co-coordination of the two ligands, and its crystal structure, decomposition temperature, sensitivity and detonation performances were tested or predicted. It was proved that the double ligand could improve the thermal stability of E-MOFs, and a new method for preparing heat-resistant energetic materials was developed.

SHI Qing-rong, SU Hui, LI Ya-qiong, DING Ning, ZHAO Chao-feng, LI Sheng-hua, PANG Si-ping

Chinese Journal of Energetic Materials (Hanneng Cailiao), 2020,28(7):609-617

Preparation and Properties of Red Pyrotechnic Colorant MOF $[Sr_2(DTDA)(H_2O)_6]_n$



ZHOU Jin-yang, HE Liu, WANG Ting-wei, ZHU Shun-guan, ZHANG Qi

Chinese Journal of Energetic Materials (Hanneng Cailiao), 2020,28(7):618-624

A novel two-dimensional energetic MOF $[Sr_2(DTDA)(H_2O)_6]_n$ (1) with high thermal stability and insensitivity was designed and synthesized by using the novel mixed ligand of high-nitrogen content and carboxylic acid H₂DTDA 2, 2'-(3, 3'-azo-bis(1*H*-1, 2, 4-triazol-5-yl)) diacetic acid and strontium hydroxide octahydrate under hydrothermal condition. 2020,28(7):625-631

Synthesis, Structure and Properties of 5,6-Diaminofurazano[3,4-b]pyrazine-4,7-dioxide



LIU Ning, DUAN Bing-hui, LU Xian-ming, ZHANG Qian, WANG Bo-zhou Chinese Journal of Energetic Materials (Hanneng Cailiao),

Synthesis and Properties of 3, 3'-Bis (2-nitroamino-1, 3, 4-oxadiazol-4-yl)-5,5'-linked-1,2,4-oxadiazole and Its Energetic Salts

A novel insensitive energetic material, 5,6-diaminofurazano [3,4-b]pyrazine-4,7-dioxide (DAFPO) was synthesized and fully characterized. The impact and friction sensitivities were measured by BAM method. The detonation velocity and pressure were calculated by EXPLO5 code.



Guided by the idea of these multicyclic compounds with a 1,2,4-oxadiazole core will have good thermal stability and high density because of their 3,5-substitution pattern and the possibility of achieving a planar conformation. Synthesis and characterization of new multicyclic oxadiazoles, 3,3'-bis(2-nitroamino-1,3,4-oxadiazol-4-yl)-5,5'-linked-1,2, 4-oxadiazole (BNOBO).



A new energetic ionic salt of 5,5'-diamino-4,4'-dinitroamino-3,3'-bi-1,2,4-triazole triaminoguanidinium salt (TAGAT) was obtained through a three-step synthesis with its crystal structure fully characterized by X-ray diffraction analysis. The thermal behaviors and detonation properties were investigated. TAGAT exhibits excellent gas-generating capability, average venting rate and good detonation performances, making it a potential gas generating compound and a promising candidate of insensitive energetic material.

LIAO Si-cheng, DENG Mu-cong, SONG Si-wei, JIN Yun-he,
LIU Tian-lin, ZHANG Qing-hua
Chinese Journal of Energetic Materials (Hanneng Cailiao),
2020,28(7):632-637

Crystal Structure and Detonation Performance of 5,5'-Diamino-4,4'-dinitroamino-3,3'-bi-1,2,4-triazole Triaminoguanidinium Salt (TAGAT)

XUE Yu-bing, CHENG Guang-bin, YANG Hong-wei
Chinese Journal of Energetic Materials (Hanneng Cailiao),
2020,28(7):638-643

Synthesis, Crystal Structure and Properties of 2-Azido-6-methyl-5-nitro-pyrimidin-4(3H)-one(AMNP)



HU Yong, YANG Jun-qing, ZHANG Jian-guo Chinese Journal of Energetic Materials (Hanneng Cailiao), 2020,28(7):644-649

Synthesis and Properties of Energetic Plasticizer Bis (3-azido-2,2-bis (azidomethyl) propyl) malonate 2-Azido-6-methyl-5-nitro-pyrimidin-4(3H)-one was synthesized via cyclization and nitration reactions by using 5-amino-1*H*-tetrazole and ethyl acetoacetate as raw material. Its structure was confirmed by elemental analysis, X-ray analysis and ¹³C NMR. Its thermal stability and decomposition process were investigated by TG and DSC method.



ZHAO Bao-dong, JIN Guo-liang, LIU Ya-jing, GAO Fu-lei,
CHEN Bin, WANG Ying-lei, GE Zhong-xue
Chinese Journal of Energetic Materials (Hanneng Cailiao),
2020,28(7):650-656

A novel multi-azido energetic plasticizer bis(3-azido-2,2-bis (azidomethyl) propyl) malonate was designed and synthesized. As the DSC results shown, BAAMPM has a rather low glass transition temperature (-58.3 °C) and good thermal stability as well as low mechanical sensitivities. Moreover, the viscosity and glass transition temperature of BAAMPM/GAP mixtures are considerably lower than that of GAP, showing that BAAMPM has notable plasticizing effect on GAP. Synthesis and Properties of Polynitro 3,3,7,7-Tetra(trifluoromethyl)-2,4,6,8-tetraazabicyclo [3.3.0]octane



YANG Tong-tong, LIU Yang, HOU Xiao-wen, MENG Zi-hui, XU Zhi-bin

Chinese Journal of Energetic Materials (Hanneng Cailiao), 2020,28(7):657–663

Synthesis and Properties of 4-Amino-1,2,3-triazolo[4,5-e] furazano[3,4-b]pyrazine 6-oxide Three polynitro 3, 3, 7, 7-tetra (trifluoromethyl) -2, 4, 6, 8-tetraazabicyclo [3.3.0] octanes were prepared and fully characterized. All compounds show good detonation performance and low mechanical sensitivity.



A novel high energy density material, 4-amino-1,2,3-triazolo [4, 5-e]furazano[3, 4-b]pyrazine 6-oxide(ATFPO), was designed and synthesized by the reactions of substitution, nitrification-cyclization, neutralization and *N*-amination. The thermal stability of ATFPO was tested by differential scanning calorimetry(DSC) method. The detonation properties of ATFPO were predicted.

LI Ya-nan, HU Jian-jian, CHEN Tao, WANG Bin, CHANG Pei, WANG Bo-zhou

Chinese Journal of Energetic Materials (Hanneng Cailiao), 2020,28(7):664-669

Stability of Oxadiazole Nitramide Compounds in Water and Its Hydrolysis Mechanism



ZHANG Zhen-qi, MA Qing, LU Huan-chang, LIAO Long-yu, FAN Gui-juan

Chinese Journal of Energetic Materials (Hanneng Cailiao), 2020,28(7):670-677

Through the theoretical calculation of NBO charge distribution and LUMO orbital distribution of oxadiazole nitramide compounds and the experimental verification of the hydrolysis reaction, the mechanism and internal rule of the hydrolysis reaction of oxadiazole nitramide compounds were revealed.

Synthesis and Properties of 1, 2-Bis (5, 5'-dinitramino-1, 3, 4-oxadiazol-2-) ethane



MA Ying-jie, LU Yan-hua, CAO Yi-lin, HE Jin-xuan Chinese Journal of Energetic Materials (Hanneng Cailiao), 2020,28(7):678-684 A new energetic compound of 1,2-bis(5,5'-dinitramino-1,3, 4-oxadiazol-2-)ethane was obtained through a three-step reaction. The mechanism of cyclization reaction was studied by quantum chemical calculation method. The thermal behaviors and detonation properties were investigated. A Melt-cast Explosive 3-Azido-1, 3-dinitroazetidine (AzD-NAZ) with Gem-azidonitro of Novel Energetic Group: Synthesis and Performance



Using (1-tert-butyl-3-nitroazetidin-3-yl)methanol as starting material, a melt-cast explosive of 3-azido-1,3-dinitroazetidine (AzDNAZ) with novel gem-azidonitro energetic group was obtained through an improved azidation-salinization-nitration strategy. Structures of the intermediates and AzD-NAZ were characterized. One of the intermediates, 1-tertbutyl-3-azido-3-nitro-azetidinium nitrate (compound 2), was obtained for the first time with the single crystal determined by X-ray single crystal diffraction. Performance of AzDNAZ was studied using DSC-TG and quantum chemical calculations.

JIA Si-yuan, ZHANG Hai-hao, ZHANG Jia-rong, LIU Qian, LUAN Jie-yu, BI Fu-qiang, WANG Bo-zhou

Chinese Journal of Energetic Materials (Hanneng Cailiao), 2020,28(7):685-689

Kinetics of Thermal Decomposition of 2, 4, 6-Trinitro-3, 5-Difluorophenol



YANG Lei, LIU Yu-cun, JING Su-ming Chinese Journal of Energetic Materials (Hanneng Cailiao), 2020,28(7):690-694 The thermal decomposition kinetics of 2, 4, 6 - trinitro - 3, 5 - difluorophenol was studied by TG-DTA method. The pre-expoential factor and apparent activation energy were calculated, and the related thermodynamic parameters were obtained.

Review on Energetic Compounds Based on Bipyrazoles: Synthesis and Property



LUO Yi-fen, XIAO Chuan, BI Fu-qiang, LI Xiang-zhi, WANG Zi-jun,	
WANG Bo-zhou	Advances in the construction of bipyrazole energetic com-
Chinese Journal of Energetic Materials (Hanneng Cailiao),	pounds were reviewed. The reported bipyrazole energetic
2020,28(7):695-706	compounds were divided by different bonding modes.
Review on Preparation of Boron-based Energetic	
Compounds	
	Five categories of boron-based energetic compounds were
	introduced and the research progress was reviewed towards
	their structural characteristics, synthesis routes and basic
WANG Guo-dong, LIU Yu-cun, JING Su-ming, LIU Guo-qing,	properties. It can be considered as a new way to improve
HAN Rui-lian	the combustion performance of fuel-rich propellants by re-

Chinese Journal of Energetic Materials (Hanneng Cailiao), 2020,28(7):707-716

n propellants by р placing boron particles. As a non-chlorine energetic material, it can also be explored to replace ammonium perchlorate.

Executive editor: WANG Yan-xiu JIANG Mei GAO Yi

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