Density Functional Theory Study on Polynitropyridines

LI Jin-shan, HUANG Yi-gang, DONG Hai-shan, YANG Guang-cheng *Hanneng Cailiao*, 2003, 11(4): 177

Underwater Shockwave Performance of Explosives

Yü Tong-chang, WANG Xiao-feng, WANG Jian-ling Hanneng Cailiao,2003,11(4): 182

Experimental Study on the Deflagration to Detonation Transition for Granular HMX, RDX

Polynitropyridines have been investigated at the B3LYP/6-31 ++ G^{**} level. Calculated results show that Mulliken population analysis is not suitable for the calculation of atomic charges of polynitropyridines, but natural population analysis can be applicable for it. It has been predicted that 3,5-diamino-2, 4,6-trinitropyridine may be a high density,low-sensitive explosive.

(NO₂)_m 019.ch (1315.019.kh (NH)、 法 指托林林

Performance with the velocity and pressure of detonation, as well as the relationship of the shockwave peak pressure with the charge and the distance to measure point, have been deeply studied. The measured results of the underwater shock energies of several explosives are presented.



ZHAO Tong-hu, ZHANG Xin-yan, LI Bin, ZHAO Feng Hanneng Cailiao, 2003, 11(4): 187

The Research of Effective Pressure and Energyreleased Process of Al-containing Explosives

HAN Yong, HAN Dun-xin, LU Xiao-jun, HUANG Yi-ming, HE Bi, GUAN Li-feng Hanneng Cailiao, 2003,11(4); 191 The experimental results show that the process of deflagration to detonation transition for the granular HMX, RDX is very complicated. It is affected by the ignition method, the impurity in the explosive and the DDT tube material.



The tracks of shock velocity were compared and analyzed in PMMA. Two types of Al-containing explosives were investigated. One was that the ratio of RDX/AP increased, while Al content kept constant. The other was that Al content increased, while the ratio of RDX/AP kept constant. NNN

Decomposition of TNT by Heat and Shock

Martin Kouba, Svatopluk Zeman, Eva Zemanová Hanneng Cailiao, 2003, 11(4): 194

Study on the Curing of EMCDB Propellant Shaped by Granule-casting Process

LI Xiao-jiang, LIU Fang-li, FAN Xue-zhong, QIANG Jie-bing, LIU Chun Hanneng Cailiao,2003,11(4): 197

Experimental Studies on the Degradation of TNTcontaining Wastewater by Ozone Oxidization Samples of technical TNT exposed to heat or to shock have been analyzed by means of high performance liquid chromatography (HPLC). It was found that the main decomposition products are identical in the two cases. It has been stated that the chemical micro-mechanism of the primary fragmentations of shocked TNT molecules should be the same as in the case of their low-temperature thermal decomposition.

The effects of various factors on the curing of EMCDB propellant, such as the resolvability of polymer binder in NG, the reactive activity of curing agent, and the sensitivity of curing reaction to combustion catalyst, were thoroughly studied. The better the resolvability is, the more completely the polymer binder is plasticized and resolved. The low reactive activity of curing agent is advantageous to form perfect cross-linking network. Only those combustion catalysts, which are weakly sensitive to the curing reaction, can be used in EMCDB propellant.

The ozone oxidizations of TNT include direction and indirection oxidizations, which respectively are the reactions between TNT with ozone and with hydroxyl, and their rates are controlled by pH. During the ozone oxidization of TNT, trinitrobenzene-like by-products (except TNT) were formed and accumulated in the wastewater with pH below 8, but in the wastewater with pH = 11, these by-products were not monitored. Rising pH, lowing TNT concentration and adding pH buffer are useful measures to increase the TNT removal efficiency by ozone oxidization. Therefore, ozone oxidization process is expected to be suitable for treating the TNT wastewater with higher pH and lower concentration of TNT.

WU Yao-guo, ZHAO Da-wei Hanneng Cailiao,2003,11(4): 201

Unsymmetrical Dimethylhydrazine Wastewater Treatment by Catalytic Reduction Process

WANG Xuan-jun, LIU Xiang-xuan, WANG Ke-jun, HUANG Xian-xiang *Hanneng Cailiao*, 2003, 11(4): 205 $2\text{Al} + 2\text{NaOH} + 2\text{H}_2\text{O} \longrightarrow 2\text{NaAlO}_2 + 3\text{H}_2 \uparrow$ $(\text{CH}_3)_2\text{NNH}_2 + [\text{H}] \xrightarrow{\text{Ni}} (\text{CH}_3)_2\text{NH} + \text{NH}_3$

This paper studies the treatment of unsymmetrical dimethylhydrazine wastewater in Ni-Al-OH⁻ system by catalytic reduction process. The reasonable technological conditions are acquired by orthogonally designed experiments.

Mechanical Sensitivity and Explosive Performance of Nitroguanidine(NQ)-based Composite Explosives



DUAN Wei-dong, Lü Zao-sheng Hanneng Cailiao,2003,11(4): 209

Synthesis of N, N'-Bis(3-chlorophenyl) - 3,4-diaminofurazan

The effects of crystal form of NQ-based composites on their explosive performances were studied. The result shows that the safety of various ordnances could be improved, and the explosive power could be remained when composite B is substituted with NQ97 – a NQ-based composite.



WANG Jian-long, OU Yü-xiang, CHEN Bo-ren, LIU Jin-quan, Lü Lian-ying *Hanneng Cailiao*,2003,11(4): 213

Analyzing the Gases Released from Aged JOB Explosives by Using Solid Phase Microextraction Coupled with GC/MS

YANG Xiu-lan, XU Rui-juan, HUANG Li-ming, Yü Kun, LI Zhe, LIU Ning Hanneng Cailiao,2003,11(4): 215 This paper describes the synthesis of N, N'-bis(3-chlorophenyl)-3,4-diaminofurazan(BCPDAF). The structures of the target compound and its intermediate were identified by IR,¹HNMR,MS and elemental analysis.

Three kinds of adsorbant solid phase microextractions (SPME) were used to study the gases released from aged JOB explosives. The extraction and adsorption properties of these SPMEs and the qualitative identification of the gas components have been examined by using SPME coupled with GC/MS analytical techniques.

Study on the Desensitization of CL-20 with TATB

XU Rong, TIAN Ye, LIU Chun Hanneng Cailiao,2003,11(4): 219 TATB has been used to desensitize the sensitivity of CL-20. Experimental results show that the desensitizing effect is better with CL-20 particles being larger and TATB particles smaller. It has been discovered that the mechanism that TATB desensitizes CL-20 is that a layer of TATB is formed on the surface of CL-20 particle.

Nitration of Tetraacetyldibenzylhexaazaisowutzitane with Phase Transfer Catalysts



PANG Si-ping, Yü Yong-zhong, ZHAO Xin-qi Hanneng Cailiao,2003,11(4): 222

Hartree-Fock Calculation of Nuclear Quadrupole Coupling Constants for ¹⁴N in RDX

SHI Guang-ming, XU Geng-guang,
WANG Ting-zeng, SONG Hua-fu, LI Run-hua
Hanneng Cailiao, 2003, 11(4): 224

Development on Some New Insensitive Individual Explosives Abroad This paper describes a new method of the nitration of tetraacetyldibenzylhexaazaisowutzitane. Tetraacetyldinitrohexaazaisowutzitane could be obtained in 66% yield.

The calculated nuclear quadrupole coupling constants for the three 14 N nucleus in the ring of RDX are 5. 671,5. 808 and 5. 838 MHz, and the asymmetry parameters 0. 545,0. 560 and 0. 564, respectively, approaching the corresponding experimental values.

WANG Zhen-yü Hanneng Cailiao, 2003, 11(4): 227

Progress in High-nitrogen Energetic Materials Derived from Tetrazine and Tetrazole The syntheses and performances of some new insensitive individual explosives are introduced, including nitro-compound explosives FOX-7, LLM-105, MTNI, 4, 6-nityoanilinodinitrobenzofuroxans, PL-1, LLM-116, ANTZ, nitramine explosives I-RDX, TEX and other explosives DAAT, DAAF, DAAzF.

This paper summarizes the research on high-nitrogen energetic materials derived from tetrazine and tetrazole recently. Their synthesis and application, which showed good foreground on insensitive explosives, low signature propellants, gas generants and low – smoke pyrotechnics, are briefly introduced.

The prospect of applying for conductive polymers and related propellants is

also discussed.

YANG Shi-qing, YUE Shou-ti Hanneng Cailiao,2003,11(4): 231

Progress in Studies on Benzofuroxan Compounds

ZHOU Hong-ping, DONG Hai-shan, HAO Ying Hanneng Cailiao, 2003, 11(4): 236 The chemical structures, syntheses, properties, and applications of benzofuroxan compounds are reviewed.

Executive editor: ZHENG Xue; Computer typesetter: LI Shao-hui