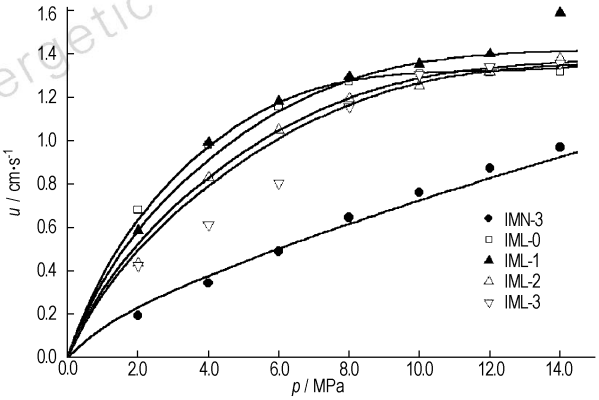
Laser Initiation of Complex Perchlorates of *d*-Metals With Heterocyclic Ligands

Mikhail A. Ilyushin, Igor V. Tselinsky, Irina V. Bachurina, Emil Ya. Seidov, Anatolii S. Kozlov, Dmitrii V. Korolev, Alexei E. Olenin

Chinese Journal of Energetic Materials, **2006, 14(6): 401 – 405**

Laser initiation for several *d*-metal perchlorate complexes with 3-hydrazino-4-amino-5-R-1,2,4-triazoles as ligands (where R = H, CH_3, SH) were investigated.

Numerical Simulation for Combustion Characteristics of Insensitive Propellant Containing Trimethylolethane Trinitrate (TMETN)



ZHAO Feng-qi, XU Si-yu, YI Jian-hua, GAO Hong-xu, SONG Hong-chang, LI Shang-wen

Chinese Journal of Energetic Materials, **2006, 14(6): 406 – 410**

The burning rates of insensitive propellant containing trimethylolethane trinitrate (TMETN) have been studied by numerical simulation and experiment. And the results obtained by the two methods are basically coincident.

Synthesis and Characterization of Poly BAMO Suitable for Binder Application

M. V. Maheshkumar, M. J. Joseph, K. Sreekumar, H-G. Ang

Chinese Journal of Energetic Materials, **2006, 14(6): 411 – 415**

A new synthetic methodology has been developed for the synthesis of poly BAMO and poly BAMO-co-THF with controlled molecular weight and narrow molecular weight distribution. Computational evaluation of the energy releasing properties of the poly BAMO derivatives was performed using Gaussian algorithm.

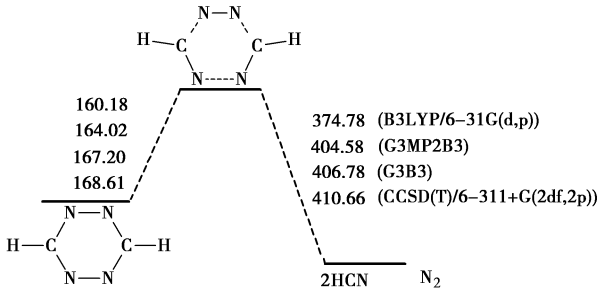
Energy Characteristics of Several Propellants With Insensitive and Minimum Signature Properties

XU Si-yu, ZHAO Feng-qi, LI Shang-wen, GAO Hong-xu, YI Jian-hua, GAO Yin

Chinese Journal of Energetic Materials, **2006, 14(6): 416 – 420**

The energy characteristics of monopropellants and propellants with insensitive and minimum signature properties containing seven kinds of insensitivity materials, such as *N*, *N*′-dinitropiperazine (DNPZ), *N*-guanylureadinitramide (FOX-12), 1,1-diamino-2,2-dinitroethylene (FOX-7), insensitivity RDX (I-RDX), 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105), nitroguanidine (NQ) and 1,4,5,8-tetranitro-1,4,5,8-tetraazadecalin (TTNZ), are calculated by propellant energy calculation program.

Thermal Decomposition Mechanism of *s*-Tetrazine by *ab* Initio Molecular Dynamics and Density Functional Theory

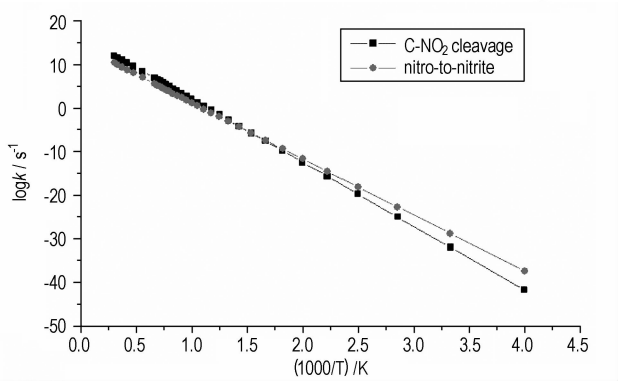


XIONG Ying, SHU Yuan-jie, ZHOU Ge, WANG Xin-feng, TIAN An-ming

Chinese Journal of Energetic Materials, **2006, 14(6): 421 – 424**

The thermal decomposition mechanism of *s*-tetrazine was studied and the reaction channel and the zero-point-corrected energy barriers (in $kJ \cdot mol^{-1}$) were obtained by combination of *ab* initio molecular dynamics method and density functional theory.

Theoretical Study on the Initial Thermal Decomposition and Catalysis Effects of NO_2 on FOX-7

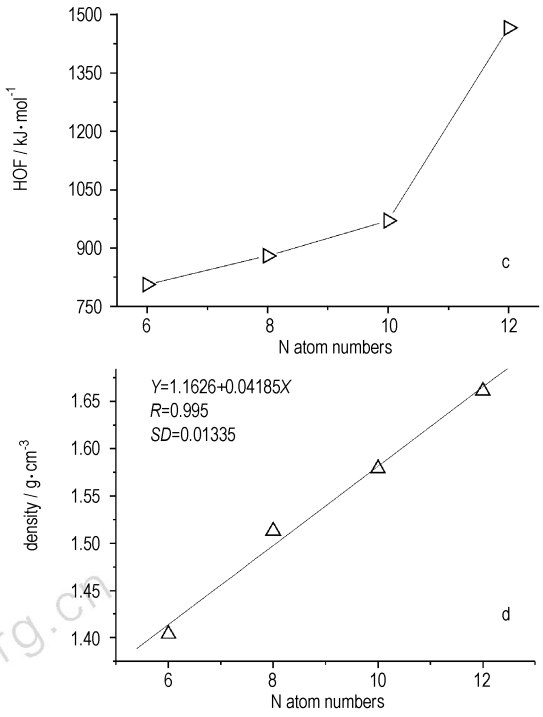


ZONG He-hou, SHU Yuan-jie, HUANG Yi-gang, WANG Xin-feng

Chinese Journal of Energetic Materials, 2006, 14(6): 425 – 428

The rate constants of C—NO_2 cleavage and nitro-to-nitrite rearrangement were studied at G3MP2B3 energy level in the range of 250 – 3300 K.

DFT Studies on the Tetrazine Substituted by Six-membered C—N Heterocyclic Derivatives

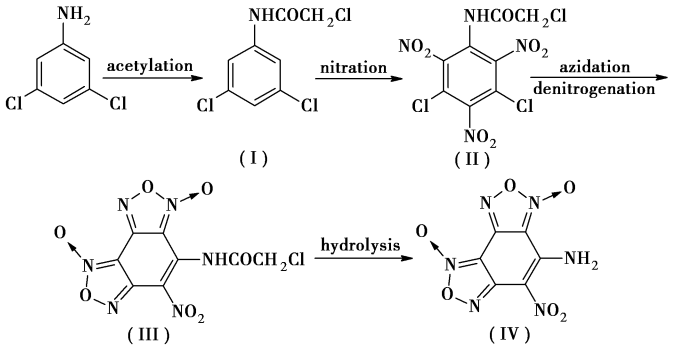


ZHOU Yang, LONG Xin-ping, SHU Yuan-jie, WANG Xin, TIAN An-min

Chinese Journal of Energetic Materials, 2006, 14(6): 429 – 435

22 Tetrazines substituted by six-membered C—N heterocyclic derivatives have been investigated by density functional theory. Their optimized geometry structures, electronic structures, conjugation, molecular energies, heats of formation (HOF) and density (ρ) were calculated at the B3LYP/6-311G(d,p) level.

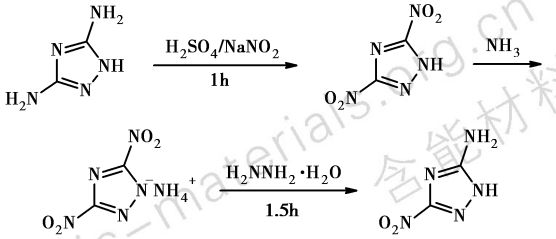
New Method for Synthesis of 7-Amino-6-nitrobenzodifuroxan



LU Lian-ying, WANG Jian-long, CHANG Yong-fang, ZHAO Jian-lu

Chinese Journal of Energetic Materials, 2006, 14(6): 436 – 438

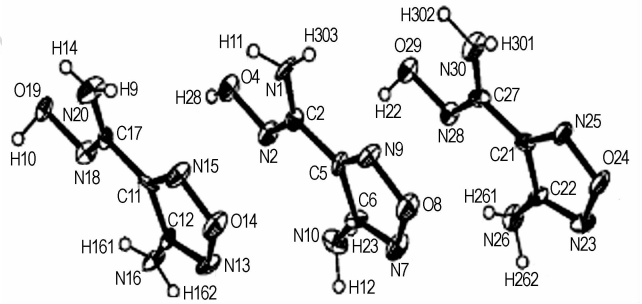
Synthesis Improvement of 5-Amino-3-nitro-1, 2, 4-triazole (ANTA)



WANG Xi-jie, JIA Si-yuan, WANG Bo-zhou, LIAN Peng, ZHOU Cheng

Chinese Journal of Energetic Materials, 2006, 14(6): 439 – 440

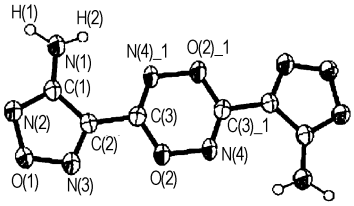
Crystal Structure of 3-Amino-4-acylaminoximinofurazan



WANG Jun, DONG Hai-shan, HUANG Yi-gang, LI Jin-shan

Chinese Journal of Energetic Materials, 2006, 14(6): 441 – 445

Crystal Structure of 3, 6-Bis(3′-aminofurazan-4-yl)-1, 4-dioxa-2, 5-diazacyclohexa-2, 5-diyne



WANG Jun, DONG Hai-shan, HUANG Yi-gang, LI Jin-shan

Chinese Journal of Energetic Materials, 2006, 14(6): 446 – 448

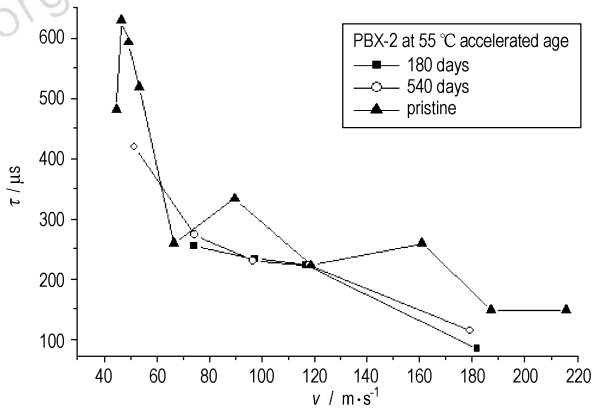
An Alternative Method for Estimation of Gurney Velocity Based on Assumed Detonation Products

A new method for prediction of Gurney velocity of explosives is introduced with assumption that the CHNO explosive reacts to form products composed of N_2, CO, H_2O, CO_2, H_2, O_2 and C(s) as determined by the oxygen balance of the unreacted compound.

Mohammad Hossein Keshavarz

Chinese Journal of Energetic Materials, 2006, 14(6): 449 – 452

Reaction Ability of PBX-2 Before and After Accelerated Aging by Projectile Impact (Steven Test)



PBX-2 explosive for 55 ℃ accelerated age 180 days and 540 days are tested in Steven test by using a steel projectile of 2.0 kg. In the test the reaction overpressures are gained by blast pressure gauges. The results primarily show that there is not obvious change for the reaction degree of pristine and accelerated aged PBX-2 explosive in Steven test.

DAI Xiao-gan, XIANG Yong, SHEN Chun-ying

Chinese Journal of Energetic Materials, 2006, 14(6): 453 – 456

Review on Synthesis of High-nitrogen Energetic Compounds

HUANG Ming LI Hong-zhen LI Jin-shan

Chinese Journal of Energetic Materials, 2006, 14(6): 457 – 462

The usual synthesis methods of HNECs, and the synthesis route of some typical HNECs were reviewed, and the some ideas on study of HNECs were suggested.

Review on 3,4-Bisnitrofurazanfuroxan (DNTF)

ZHENG Wei, WANG Jiang-ning

Chinese Journal of Energetic Materials, 2006, 14(6): 463 – 466

The physicochemical and thermolysis properties of 3,4-dinitrofurazanfuroxan (BNFF or DNTF), and its applications in the explosive composition, CMDB and related items were reviewed.

Progress in High Energetic Explosive: TEX

LEI Yong-peng, XU Song-lin, YANG Shi-qing, ZHANG Tong

Chinese Journal of Energetic Materials, 2006, 14(6): 467 – 470

Progress in study on high insensitive explosive compound, 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazaisowurtzitane (TEX) was reviewed. Its excellent characteristics shows that TEX has good potential applications as explosive composition.

Safe Preparations of Fine Ammonium Perchlorate Particles

Makoto Kohga

Chinese Journal of Energetic Materials, 2006, 14(6): 471 – 474

Some safe methods for preparing the fine spherical, porous, and hollow AP particles including spray-dry method, freeze-dry method, the crystal habit modified AP particle were reported.

Development on Nitrogen Heterocyclic Energetic Compounds

YANG Shi-qing, XU Song-lin, LEI Yong-peng

Chinese Journal of Energetic Materials, 2006, 14(6): 475 – 484

Progress in the synthesis and performance research of new nitrogen heterocycles energetic compounds including furazan, trizole, trizine, tetrazole, tetrazine, polycyclic cage and all-nitrogen compounds etc. was reviewed and discussed.

Structure Analysis, Solubility and Thermodynamics Properties of Adamantane

LIU Sa, GUO Jian-wei

Chinese Journal of Energetic Materials, 2006, 14(6): 485 – 490

The molecular structure and crystal phase transfer of adamantane determined by XRD, FT-IR, MS, NMR, EMS, DMS, RAMAN, DSC, etc were introduced. The thermodynamic properties and solubility of adamantane in various of organic solvents were reviewed respectively. The latest research progress of polynitroadamantanes and polynitroazaadamantanes in HEDM molecular design were also illustrated.

Study on Two Coordination Compounds Using Semicarbazide (SCZ) as Bidentate Ligands: $[Ni(SCZ)_3](NO_3)_2$ and $Cu(SCZ)_2Cl_2$

GUO Jin-yu, MA Gui-xia, ZHANG Tong-lai,
ZHANG Jian-guo, LIU Yan-hong

Chinese Journal of Energetic Materials, 2006, 14(6): 491

Two kinds of coordination compounds, $[Ni(SCZ)_3](NO_3)_2$ and $Cu(SCZ)_2Cl_2$, have been prepared by direct methods using semicarbazide as starting material. And their crystals were cultured at room atmosphere and their stuctures were identified by X-ray single crystal diffraction.

Particle Qualities of D-RDX

HUANG Ming, LI Hong-zhen, XU Rong, LI Jin-shan, NIE Fu-de, HUANG Hui, ZHANG Ming, HAN Yong

Chinese Journal of Energetic Materials, 2006, 14(6): 492

The particle qualities of D-RDX obtained with special crystallization technique, were studied. And the effects of D-RDX and normal RDX particle qualities on the shock wave sensitivity were studied by using small scale-gap test. The results show that decrease level of the shock wave sensitivity of D-RDX is equal to that of SNPE I-RDX and Australia Grade A RDX.

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