Abstracts of the 21st Seminar on

New Trends in Research of Energetic Materials

NTREM

Pardubice, April 18–20, 2018

University of Pardubice, Faculty of Chemical Technology
Institute of Energetic Materials

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New Trends in Research of Energetic Materials

Held at the University of Pardubice

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Intended as a meeting of students, postgraduate students, university teachers, and young research and development workers, concerned from the whole world.

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Preface

The original purpose of our NTREM Seminars was to allow young scientists from the field of energetic materials to present their work in English in front of scientific audience and gain the necessary confidence needed for their carrier growth. On the basis of the comments and advices thus obtained, the young incoming scientific generation could correct their approaches and results and then publish the results in scientific journals. In agreement with the above-mentioned, the Central European Journal of Energetic Materials has been also established in 1994, which is issued by the Institute of Industrial Organic Chemistry in Warsaw. I hope that the original aim of our meetings is thus being achieved.

This year's Seminar NTREM, the 21st meeting in order, is the 20th one for Institute of Energetic Materials (IEM). It seems that the number of attendees of these meetings has stabilized by the 2017 between of 180–200 participants from 24–27 countries. From the time of the 8th Seminar NTREM, the best lectures and the best posters of young authors are evaluated. An overview of numbers of thus awarded contributions the following table presents.

Country	Lectures	Posters
Germany	9	14
Russia	8	8
UK	7	2
Czechia	4	5
Poland	1	4
USA	2	0
Korea	0	2
China	1	2
India, Israel, Singapore Sweden, Belgium	1	0
South Africa	0	1

Of course, that abundance in attendance of authors from individual countries has own influence here, nevertheless, it is possible to say here that the German successes were achieved mainly by Ph.D. students of Prof. Klapötke (LMU Műnich), the Russian ones were mostly received by young scientists from the Zelinskii Institute of Organic Chemistry in Moscow. Also thanks to them, our Seminars are attractive for the general public from the area of the theory and technology of energetic materials.

It is well known that our Seminars are non-profit with strong emphasis on suppression of oral commercial presentations and they serve mainly to the young scientists and students in their introduction into the field of science of energetic materials. It means that the existence of these meetings depends on financial support of external organizations. This year's Seminar is traditionally, sponsored by number of institutions and individuals enabling attendance of wide range of participants, including students and young researchers not yet well financially covered by research grants. For this support we would like to thank all of our sponsors that have decided to support us again this year:

Austin Detonator, Vsetin, Czech Republic, Explosia, Pardubice, Czech Republic, Biazzi SA, Switzerland, OZM Research, Hrochův Týnec, Czech TRepublic, Office of Naval Research Global, Science & Technology, London, US Army RDECOM—Atlantic, Nicolet CZ, Prague, Czech Republic, Tempreratior, Liberec, Czech Republic, Faculty of Chemical Technology, University of Pardubice.

The efficient help in ensuring smooth and successful course of the meeting obtained from all these institutions and also supporters from the Seminar participants is gratefully acknowledged.

The mentioned smooth course of the Seminar would not be possible without the voluntary involvement of staff of the Institute of Energetic Materials. A great work has been done traditionally by our organizing committee; thanks a lot for its perfect organization and services.

And traditionally, let mi thank to the members of the scientific committee, the authors of all the seminar papers and, last but not least, you, the participants of this seminar, for its success. I wish you big successes in your life and scientific work, a good health and hope to see you in April.

Pardubice, March 16th, 2018

Svatopluk Zeman

Making sense of sensitivity data

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Keywords: small-scale; sensitivity; explosives; impact; Bruceton; d-optimal; probit.

Sensitivity to a range of stimuli, as measured in small-scale tests, is routinely reported for new energetic materials. Often insufficient information is given for the results to be interpreted in the context of the behaviour of other energetics. This paper focuses on small-scale impact sensitivity testing and the information about the testing that is needed for a meaningful evaluation of those results to be made. The discussion addresses impact sensitivity tests, but the lessons are applicable to other types of small-scale sensitivity testing as well.

Development of performance testing at IEM

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Keywords: detonation parameters; experimental; blast wave; effects; PDV; OPTIMEX.

The Institute of Energetic Materials is a part of the Faculty of Chemical Technology and as such has throughout the decades of its existence strongly emphasized on preparation of new explosives. The organic synthesis presented the core of the scientific activity of the institute for a long time. A new modern separation, spectral and thermoanalytical techniques typical for chemical laboratories have been acquired and implemented in an everyday work done by both staff and students alike over the past couple of decades. The sensitivities of a newly prepared materials have traditionally also been tested particularly towards impact, friction and electrostatic discharge. The determination of explosive performance parameters has for a long time been based on historical methods out of which only detonation velocity was directly related to the parameters of the detonation front. Further effects were evaluated from experiments in which state of some experimental setup was observed before and after the shot. Such tests were based on creating perforation or dent in some witness plate, compressing cylinder, moving pendulum etc. The need for improvement in characterization of detonation parameters as well as effects of real size charges resulted in implementation of various newly implemented techniques. The passive as well as active fiber optical methods were developed to look at the detonation front behavior and the shocks in explosively loaded solids, various pressure gauges were tested for measurements of blast waves in air. High speed visualization techniques together with numerical methods are being employed to help in explaining the experimentally observed phenomena. This contribution concentrates on advances in performance characterization of energetic materials achieved at the institute over the past ten years.

Polycyclic amines: synthesis, property and application

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Branch of the Russian Academv of Sciences

Keywords: nitramine.

Oxaazaisowurtzitane derivatives are promising compounds that can successfully be used in military, space and medical industries. This report describes synthetic methods and new applications of these chemical entities

Exploring the effects of reactive additives in explosives: In search of higher efficiency with various energetic combinations

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Keywords: nitramine; detonation; Gurney energy.

The energy available for useful work in C,H,N and O explosive materials has for the most part plateaued with the synthesis of dense nitramines such as hexanitrohexaazaisowurtzitane (CL-20). In order to obtain higher overall energy, reactive additives can be formulated with various explosive materials, such that significant gains can be obtained. Powdered aluminum is a common additive to energetic materials, but little is understood regarding its reaction rate at very high temperatures as well as high pressures in specific oxidizing gases such as carbon dioxide or water. When looking at other materials such as Si, B, physical mixtures and alloys, even less is understood, due to difficulties in the study of particulate oxidation at the high pressures and temperatures in detonation reactions. To study these reactions, small particle size reactive materials (Al, B, Si, Al/PTFE and MgB) or the inert surrogate, LiF, was added to various energetic material including HMX, CL-20, benzotrifuroxan (BTF) and hydrazinium nitrate/hydrazine eutectic and performance of the formulations were evaluated. High-fidelity detonation velocity diagnostics were utilized to determine reactive material contribution in the detonation reaction zone and PDV measurements were utilized to determine contribution in the expanding product gases via early wall velocity expansion measurements in 12.7 mm copper cylinders. Both thermal equilibrium calculations and solution of the JWL equation of state were used determine temperature, pressure and energies at specific time periods, in addition of Gurney energies, which enables the elucidation of reactive material reaction extent. Comparison of this oxidation with the inert formulation data indicates that oxidation can occur on an extremely fast time scale, beginning and completing between 1 and 25 microseconds in some cases.

Prediction of regulation toxicological tests applied to high energy molecules

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Keywords: toxicology; algorithm; HEM.

In collaboration with Ariane Group, a research program was set up to have, in the future, optimized tools to predict the toxicity of High-Energy Materials (HEM). The European Union has adopted a legislation about chemicals named REACh (Registration, Evaluation, Authorization and Restriction of Chemicals) to ensure a high level of protection of human health and environment. REACh describes the internationally guidelines of the different toxicological tests like the Ames test for example. Several in silico methods can be used to predict the toxicity of molecules such as machine learning. The search of structural similarity among molecules is one of the most conventionally used tools in the in silico predictions. Databases used in this study compiled available data on mutagenicity, carcinogenicity and reprotoxicity for a lot of diversified molecules. An explicit list of explosives, from which we know the experimental results for the different toxicological test in the literature, has been chosen to consolidate the predictive system and validate the predictions. All these compounds were evaluated for evidence of potential toxicity. The goal of this study is to use a smarter algorithm, previously developed at the PRABI-LG, to investigate the use of similarity indices. The prediction is performed implemented in Python language in order to obtain an efficient prediction tool for different kind of HEMs. This prediction tool will be compared with softwares often used in the scientific community such as ACD. This phase allows assessing the prediction's quality. The subject of this paper is to show that our similarity tool can be encoded and applied itself to a wide range of different similarity indices for the prediction of activity of chemical compounds.

The connection between WLF equation and the Arrhenius equation

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Keywords: WLF equation; Arrhenius equation modified; Arrhenius equation; parameter connection WLF-Arrhenius.

The description of the change of thermomechanical and viscoelastic properties of polymers and elastomers with deformation frequency is widely achieved by two equations: (1) the Williams-Landel-Ferry (WLF) equation and (2) the Arrhenius equation. Mostly the WLF equation is used. Often the distinction between the two descriptions is based on the argument: if volume processes play the key role then WLF equation is right one, if thermal processes play the key role then Arrhenius equation is the right one. Both equations are based on the activation of processes, here intermolecular volume change and overcoming of intermolecular interaction energies. Always the temperature is the variable, which activate the processes. Also, the so-called volume processes are controlled by temperature. This means both descriptions should be congruent. In this contribution, the congruence is shown and the relation between WLF parameters and Arrhenius parameters will be established. For this, a slight modification of the usual Arrhenius equation is necessary, and a modified Arrhenius equation is introduced. Applications of the modified Arrhenius equation in comparison with standard Arrhenius equation and the WLF equation are discussed.

Triazanes and their reactivity: a new trend in polynitrogen chemistry

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Keywords: triazane; polynitrogen; HEM.

Triazanes and their reactivity: a new trend in polynitrogen chemistry Thomas CRITON, Lionel JOUCLA, Guy JACOB & Emmanuel LACÔTE

The Hydrazine and Energetic Materials Laboratory is known for years for its work on hydrazines and derivatives. Back in 90's, the success of the well-known "Raschig" process for the industrial synthesis of monomethyl hydrazine (MMH) and unsymmetrical dimethylhydrazine (UDMH) have enabled the production of large amounts of propellants to provide spatial industry. Even if hydrazines are still used nowadays, these compounds happened to be very toxic for both human and environment. The general aim of our laboratory is to expand the chemistry of these molecules to higher polynitrogen systems to increase performances and lower harmfulness. Among the work carried out in our laboratory, triazanium salts have been compounds of interests due to their very interesting properties for solid propellant. Nevertheless, researches on neutral triazanes for liquid propulsion has been recently at the centre of our attention, with the objective to synthesize polynitrogen homologues of hydrazines with higher performances. This work will be based on our laboratory know-how in the synthesis of these compounds.

The synthesis and a physicochemical study of new triazanes will be presented. Furthermore, a work on reactivity (deprotonation, alkylation, . . .) of N3 patterns will be detailed to show the potential of such structures as precursors for new polynitrogen systems.

Preparation and characterization of ε-HNIW by solvent/anti-solvent recrystallization

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Keywords: HNIW; recrystallization; purity; morphology; crystal size distribution.

In order to obtain the desired morphology and crystal size distribution (CSD) of the crystal for the application of composite explosive. The ε-HNIW was successfully precipitated using solvent/anti-solvent method with technical grade solvents. The chemical purity, polymorphic purity and morphology of the recrystallized products and raw HNIW were analysed and compared by the means of High Performance Liquid Chromatography (HPLC), Powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), optical microscopy (OM). The crystal apparent density, CSD and impact sensitivity were also measured. The results showed that there is no significant difference between the recrystallized HNIW and raw HNIW, except for the morphology, crystal size distribution, and impact sensitivity. After recrystallization, the morphology of the crystals changed from dominantly bi-pyramidal agglomerates to block-like single crystals with smooth and integrated particle surface. The median diameter (by volume) of crystal size distribution increased from 22.4μm to 201.4μm. Compared to the raw HNIW, the impact sensitivity of the recrystallized sample significantly decreased with the drop height (H50) increasing from 25.0 cm to 42.3 cm. These controllable size distribution and morphology ε-HNIW are highly desirable for particle grade technique in HNIW-based composite explosive.

Preparation, mechanical activation and properties of the Al-Mg system powder materials

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Keywords: aluminium; magnesium; powders; mechanical activation.

The aim of the work is to obtain powder materials of the Al-Mg system, to select processing regimes and to study the properties of the obtained powders. The paper presents the results of studies aimed at obtaining powder materials of the Al-Mg system. The starting material for the powders synthesis was an alumina-magnesium alloy of 99% purity.

Mechanical activation of the powder materials was carried out in a planetary ball mill for nine hours, the processing frequency varied from 10 to 14 Hz. A study was made of the phase composition and structural parameters for the starting material and for the selected samples. Sample collection was carried out every hour for nine hours of activation process. The results of phase composition studies showed an Al / Mg phase ratio of 50 / 50%. The lattice parameters of the obtained powder materials are determined. SEM images are obtained. Dependences of the dispersion of synthesized powders on the treatment time in a planetary mill are obtained. Studies of the physico-mechanical and thermochemical properties of the resulting matrices are carried out.

A chlorine- and dichromate-free pyrotechnic strobe system for multiple colors

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Keywords: pyrotechnic strobe formulation; chlorine-free; strobe frequency.

Classical pyrotechnic strobe formulations suffer from manifold environmental issues: they use perchlorate oxidizers which in combination with organic moieties form highly carcinogenic polychlorinated aromatics; the United States Environmental Protection Agency is considering to regulate strontium compounds as traditional red coloring agents due to health concerns and intoxications from green light-producing barium compounds result in respiratory and heart problems; furthermore, many strobe formulations employ potassium dichromate in order to improve the regularity and the sharpness of the flashes but this chemical is classified as a substance of very high concern by European Chemicals Agency. The present work establishes a pyrotechnic strobe system which meets the requirement for industrial use of strobe frequencies between 1 Hz and 10 Hz, can be adjusted to various colored flame chemistries and addresses the afore-mentioned problems.

A new melt-cast energetic material of 5,6-Di(2-fluoro-2,2-dinitroethoxy)furazano[3,4-b]pyrazine facile synthesis, polycrystalline properties and promising performance

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Keywords: melt cast; crystal polymorphism.

In a sustained effort to seek more potential melt-cast energetic materials with high performance, we combined the advantages of fused furazano[3,4-b]pyrazine and bis(2-fluoro-2,2-dinitroethyl)formal (FEFO), and designed a new fluorodinitro (FDN)-based structure named 5,6-di(2-fluoro-2,2,-dinitroethoxy)furazano[3,4-b]pyrazine (FDEFP) (Fig. 1). In order to construct this new compound, we have developed a new and convenient synthetic route. FDEFP was synthesized in a three-step process starting from 3,4-diaminofurazan (DAF) including a significant nucleophilic substitution reaction under the catalytic effect of trisodium phosphate dodecahydrate (Fig. 2). The structure of FDEFP was characterized by 1H, 13C, 15N, 19F NMR spectroscopy and single-crystal X-ray diffraction. The crystal and structure data indicates that FDEFP possesses a higher crystal density than that of 2,4,6-trinitrotoluene (TNT) at ambient temperature. Interestingly, crystal polymorphism phenomenon was also observed as shown in the crystal structure analysis (Fig. 3). Single crystals of FDEFP grew from acetone (FDEFP-A) and methanol (FDEFP-M) show orthorhombic space group Fdd2 and orthorhombic space group Pca21, respectively. To investigate its polycrystalline properties, differential scanning calorimetry (DSC), powder-X-ray-diffraction (PXRD) and ab initio calculation by the Viena Ab initio simuation package (VASP) were employed. PXRD and DSC reveal that different polymorph has significant effect on their phase structure and thermal properties, respectively (Fig. 4). Moreover, the ab initio simulations of unit cell in crystal indicate that hydrogen and halogen bonding interaction in FDEFP-M is stronger than that of FDEFP-A. Important performance results show that FDEFP has realizable melt-castable properties(onset melting point at 117 °C), high decomposition temperature exceeding 200 °C and exhibits better detonation properties (D: 8512 m/s, P: 32.4 GPa) than those of TNT. Worth noting that it also indicates slightly better insensitivities (IS: 17J, FS: 252N) than those of TNT. The above-mentioned performance not only suggest that the incorporation of FDN moiety into framework with high HOF is helpful for enhancing the energetic properties but also show that performance has the potential as an ingredient in melt-cast energetic materials.

High energy catalytic studies of industry scale synthesized gamma ferric oxide (γ-Fe2O3) nanoparticles

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Keywords: industrial scale synthesis; burning rate modifier; nano metal oxide; field emission scanning electron microscopy.

Present reported research work i.e. bulk synthesis of Gamma Ferric Oxide (γ-Fe2O3) nanoparticles (NPs) and its High energy catalytic studies carried out at Research and Development Center on High Energy Materials, Premier Explosives Ltd, Secun-derabad. γ-Fe2O3 have been synthesized in bulk by using Self-Propagating Low Tem-perature Combustion Synthesis (SPLTCS) method with Ferric salt (FAS) with polyeth-ylene glycol (PEG) as a fuel. Gamma Ferric Oxide NPs were characterized by Pow-der X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Scan-ning Electron Microscopy (SEM) techniques Energy Dispersive Spectroscopy (EDAX)and Field Emission Scanning Electron Microscopy (FESEM) techniques were performed for studies of atomic/crystal arrangement, functional groups, surface par-ticle size and shape morphology study respectively from characterizations confirmed the formation of polymorphic γ-Fe2O3 nanoparticles in the range of 40 to 80 nm. High energy catalytic study observed that γ-Fe2O3 nanoparticles more efficient burn rate modifier compares to commercial Ferric Oxide.

Study on sensitivity and detonation property of explosive containing B/Al

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Keywords: explosion mechanics; explosives containing B/Al; preparation; mechanical sensitivity; detonation properties.

In order to explored the application of B/Al compound powde in energetic materials, a new HMX based explosive formulation containing B and Al powder, oxidizer AP, polyurethane binder is designed and prepared. The morphology of B, Al and B/Al compound powder is observed by SEM and the SEM images at different sizes are obtained. The impact sensitivity, friction sensitivity, electrostatic spark sensitivity, cap initiation sensitivity are measured, which made a fully acknowledge of the safety of explosive containing B/Al under different external energy stimuli. The spring electric pin method is applied to measure detonation velocities of prepared Φ50mm explosive cylinders containing B/Al. The detonation pressures are calculated by the empirical equation, the influence of B/Al compound powder content on detonation property is discussed. The results show that there are many little amorphous flake B powder on the surface of Al powder for the B/Al compound powder. The mechanical sensitivity of explosive containing B/Al is higher, while the mechanical sensitivity is obviously lowered by adding desensitized HMX and AP, and it can be further lowered by adding polyurethane binder. While the formulation PF-1, PF-2 and PF-3 are solidified by vacuum vibration casting, the densities of Φ50mm explosive cylinders are about 1.693g•cm^{-3}, the detonation velocities are between 7.800-8.000 mm•μs^{-1}, and the detonation pressures are about 24GPa. The formulation PF-3 with B/Al compound powder weight rate of 1:1 and content of 20%, the combination effect of explosive containing B/Al leads a little of B/Al compound powder to take reaction in reaction area, comparing to other formulations, the detonation velocity and detonation pressure of explosive are higher.

Chlorine-free red and yellow strobe formulations

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Keywords: strobes; chlorine-free.

Novel yellow- and red-light emitting pyrotechnical strobe formulations were developed. The developed strobe formulations are covering a frequency range of 4 < x < 20 Hz and do not apply potassium dichromate, which is frequently applied as a stabilizer. Frequency measurements and a comparison to a literature-known state-of-the-art red reference strobe formulation revealed a comparable flash separation. High-speed video recording of the burning formulations showed a difference in the dark phase reactions. In contrast to no light emission for the Sr-reference and almost no light emission in the case of the lithium-based strobes, a small yellow flame was observed in the sodium-based yellow strobe formulations. In addition, the newly developed formulations meet the requirements of the U.S. EPA (Environmental Protection Agency) and European regulation law REACH (Registration, Evaluation, Authorization, and Restriction of Chemicals), as they do not contain any substances of very high concern (SVHCs), heavy metals or chlorine atoms. All formulations were investigated regarding their combustion behaviour as well as their energetic and thermal properties.

Thermal explosion of a TATB-based aluminized explosive

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Keywords: thermal stability; cook-off; TATB; energetic material.

In this work, The TATB/Al explosive formulation (T-Al, 70wt% TATB/25wt% Al/5wt% fluorine resin) was produced by an extrusion technique and the thermal explosion behaviours were studied by differential scanning calorimeter, scaled thermal cook-off tests, and ABAQUS finite element analysis. During the heating process, no blast pressure was detected by the gauges. Combustion of the explosive was observed when the temperature was increased to 583K. The reaction degree was determined to be a burning reaction without blast or fragment damage to the surroundings, demonstrating the excellent thermal stability of T-Al. T-Al cylinders of Φ60mm×120mm, and Φ100mm×100mm, in the thermal cook-off experiments, showed almost the same runaway temperature, indicating the slight dependence of the critical response temperature (approximately 583K) on the size of the explosive cylinders in our investigated regions, which was quite different from those of the HMX-and RDX-based explosives. Prior to the thermal ignition of the explosive cylinder with size of Φ100mm×100mm, the temperatures were 584K, 544K, and 531K for the surface, 1/2 radius, and the center of the explosive, respectively. The simulated temperature profiles by ABAQUS finite element analysis was close to the measured values. The thermal ignition of T-Al occurred at the edge of the cylinder according to the experimental and numerical simulations. The critical thermal runaway temperature for T-Al was calculated based on the Semenov's thermal explosion theory and the thermal decomposition kinetic parameters of the explosive, which was consistent with the experimental value, demonstrating the reliable pre-evaluation of the thermal response of the TATB-based aluminized explosive.

A comparison of the mechanical properties of explosive simulants prepared using traditional and resonant acoustic mixing

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Keywords: RAM; mixing; processing.

Resonant acoustic mixing (RAM) is a technique that is increasingly used in the energetics community to overcome the issues associated with mixing materials of widely varying properties. This technique is a batch process, where the mixer propagates acoustic energy through a baseplate into a sealed, clamped sample vessel. In comparison to the conventional planetary mixing there are no intrusive mechanical parts and the sample is intimately mixed in a short duration of time. However, there are questions about how the high intensity mixing will affect the overall material properties and ageing characteristics. This paper is the second of a larger research project, investigating the effect of resonant acoustic mixing on energetic materials and follows on from the previous presentation made last year. It consists of a comprehensive study investigating the mechanical and thermal properties of inert compositions increasing in complexity from simple 2 component composites to a full inert mimic composition; using melamine and barium sulphate as the filler system. There are several solid loading levels; 66%, 73% and either 80% or 85%, depending on the presence of plasticisers.

On the sensitivity of tetraethyleneglycol dinitrate

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FOI

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Keywords: TEGDN; impact sensitivity; contaminates.

FOI prepared tetraethyleneglycol dinitrate (TEGDN) for evaluation in a nitrocellulose propellant. To our surprise, the product was considerably more sensitive to impact than described in the literature and also more sensitive than older batches produced at FOI a few years ago. Analysis of older batches displayed small amounts of contaminates. This led to a study on how small amounts of contaminates affect the sensitivity and how to reduce the sensitivity of the product to such an extent that it would be easy to handle. This paper describes this work, the methods used to measure sensitivity at FOI, and the efforts to harmonise such methods in Europe.

Effects of temperature and humidity on the mechanical sensitivity of firework compositions

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Keywords: Drop hammer sensitivity; fireworks.

In previous safety performance evaluations, many researchers have investigated the mechanical sensitivities (e.g., drop hammer sensitivity, friction sensitivity) of firework compositions. However, these mechanical sensitivity tests lacked reproducibility, and their results were significantly scattered in some cases. One reason for this experimental error is that the ambient temperature and humidity conditions during testing influence mechanical sensitivity. In this study, we conducted drop hammer sensitivity tests according to Japanese Industrial Standard JIS K 4810 for three types of firework compositions (black powder consisting of KNO3/C/S = 77/15/8, red colorant consisting of KClO4/MgAl/SrCO3/others = 56/11/17/16, and whistle agent consisting of KClO4/potassium hydrogen terephthalate = 71/29) under different temperature and humidity conditions. We found the compositions to be more sensitive at high temperatures (43–45 °C) than at room temperatures (23–28 °C), regardless of the type of test sample. In contrast, the effects of humidity varied depending on the type of test sample; red colorant was sensitized, and black powder and whistle agent were desensitized under highly humid conditions (77–87 rh%). This result may suggest that substances that react with water, such as MgAl in the red colorant, enhance the sensitivity of firework compositions under highly humid conditions. In contrast, highly water soluble inorganic salts, such as KNO3 in the black powder, would be desensitized by dissolving into atmospheric water.

Dinitrates of malonyl and nitraminodiacetyl hydrazides

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Keywords: energetic material; nitrate; hydrazide; hydrazine.

The hydrazides of malonic acid and nitraminodiacetic acid are used as starting materials to synthesize the corresponding dinitrates. The hydrazides can be obtained in good yields by the reaction of the carboxylic acid ethyl esters with hydrazine in aqueous media. The conversion into the nitrates was accomplished by the reaction with diluted nitric acid in a solvent mixture of ethanol and water. The new nitrates were characterized by NMR spectroscopy and elemental analysis. Densities of the salts were estimated and the thermal properties and sensitivities towards impact and friction were measured. The energetic properties were predicted with EXPLO5 utilizing heats of formation calculated with the GAUSSIAN program package.

Synthesis of nitro substituted aryl-tetrazole derivatives and energetic studies

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Keywords: tetrazole; nitration; insentitive.

Various nitro substituted-N-aryl/hetero-aryl-tetrazoles are synthesized. The nitro-rich aryl-tetrazoles are prepared by the condensation of anilines and triethylorthoformate in acetic acid followed by the cycloaddition of isocyanide intermediate with dipolar-azide and subsequent nitration. 1H and 13C-NMR spectroscopy studies characterizes these compounds. X-ray diffraction analysis confirms the structures of these compounds. Thermal properties are determined by DSC-TGA data. Heats of formation are calculated from the computational studies. The molecules exhibited density in between 1.57 to 1.79 g/cc; some of the newly synthesized compounds showed good thermal stability, high positive heats of formation, reasonable detonation velocities, and pressures.

Multi-colored smoke signals applying the concept of fuel mixes

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Keywords: smoke; pyrotechnic; fuel mix; multi-color.

Novel sugar-free multi-colored smoke formulations fulfilling the concept of so-called fuel mixes were developed. These mixtures only consisted of four ingredients: dye, potassium chlorate, 5-amino-1H-tetrazole (5-AT) and a magnesium carbonate derivative. Here, the respective fuel mix is prepared by pre-mixing all components except the dye. In a further step, any dye (Disperse Red 9, Violet Dye Mix, Solvent Yellow 33, Solvent Green 3) can be added to obtain a variety of colored smokes by applying the same pyrotechnical system. Even for producers and consumers, fuel mixes are advantageous to reduce costs and at the same time reducing the amount of potentially explosive material in stock. Previous research in our group focused on white smokes containing 5-AT as main fuel, which resulted in an overall higher smoke efficiency and persistence in contrast to sugar-based formulations. This method was applied to new 5-AT-based multi-colored smoke compositions.

Performance test of small size shaped charges

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Keywords: melt cast; shaped charge; penetration test.

This paper describes the research on testing of small size point focal shaped charges. They were manufactured from composite-B, Semtex and pressed RDX, and binary explosives, and emulsions. As the liner and the whole structure of the charges were identical the mild steel penetration test was a clear method for comparing and quantifying their performance. The target setup was also standardized with different steel discs. During testing I realized that it was a practical development tool, to find a proper mixture for binary explosives. Since most of the shaped charge literature related to their evaluation was rather detailed theoretical work, I wanted to have a simple, yet productive performance testing method that suited more to practical field works.

Study on ignition and combustion characteristics of Al/Mg fuel-rich propellant under tangential air flow

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Keywords: Al/Mg fuel-rich propellant; ignition delay time; combustion.

Solid propellant, as the power source of propulsion system, has obvious influence on the internal ballistic characteristics of ramjet engine. The ignition and combustion characteristics of solid propellant help to reveal the combustion mechanism and have important guiding significance for estimating the performance of propulsion system. In this paper, the ignition and combustion characteristics of Al/Mg Fuel-rich Propellant under tangential air flow were studied. Laser ignition experiment was carried out on the Al/Mg Fuel-rich Propellant at different tangential air flow rates and tangential air flow components. The results show that the air flow rate and air flow composition can affect the flame shape and the brightness of the propellant. At the same time, with the increase of air flow rate, the more obvious the erosion combustion effect on the propellant burning surface. The air flow rate also affects the ignition delay time. When the air flow rate is low, the ignition delay time decreases with the increase of air flow rate. When air flow rate is 0.8L/min, the ignition delay time is reduced to the minimum of 350ms, but with the air flow rate continues to increase, the ignition delay time is increasing. As the oxygen content in the air flow increases, the ignition delay time increases. However, when the oxygen content is less than 14% or higher than 21%, the effect of oxygen content on the ignition delay time is weakened.

Effect of hydrogen storage alloy with PTFE in high energy solid propellant

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Keywords: aluminium; hydrogen storage alloy; PTFE ; solid propellant; combustion.

In solid propellants, aluminium (Al) is widely used to improve combustion and specific impulse performance. It can enhance reactivity and reduce two-phase flow losses of combustion by the replacement of micron scale Al with composite fuel particle. In this paper, the effect of hydrogen storage alloy with PTFE ($M_{10}F_2$) in high energy solid propellant was characterized using scanning electron microscope, differential scanning calorimeter, adiabatic bomb calorimeter and underwater acoustic combustion speed tester. The high energy propellants containing $M_{10}F_2$ and Al were prepared by a vertical mixer. DSC-TG studies established that hydride decomposed at temperature of 570 ^{o}C in $M_{10}F_2$, which can not be observed in micron scale Al curves. It showed that melting temperature of Al can lower from 660 ^{o}C to 635 ^{o}C in GAP/$M_{10}F_2$ and catalyze decomposition of AP from 354 ^{o}C to 325 ^{o}C compared with GAP/Al/AP, which was attributed to the quicker ignition of Al, the more gaseous products of metal hydride and the oxidation of Al particles by fluorine from PTFE. Experiments were carried out in the pressure range of 3-9 MPa to determine the burning rates of cured solid propellant. The results indicated that $M_{10}F_2$ based propellant showed a pressure exponent of 0.42, which increased 8.9% in propellant burning rate at 7MPa. To investigate the combustion efficiency, the content of active Al in residue after explosion heat test and the particle size in residue after combustion were analyzed. It showed the residue of $M_{10}F_2$ based propellant had a deceasing of content of active Al after explosion heat test and a smaller particle size after combustion. It is obvious indicated that the propellant containing $M_{10}F_2$ particles results in faster and more complete Al combustion. It is concluded that the hydrogen storage alloy with PTFE exhibits an efficient replacement of micron scale Al used in high energy solid propellant.

A novel strategy for smart control by micro-scale oscillatory networks of the reactionary zones for enhanced operational capabilities of the next-generation solid propulsion systems

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Keywords: next-generation solid propulsion system; reaction zone; micro- and nano- scale oscillatory network; self-organized wave pattern; cymatic; extreme thrust control; energy-releasing areas.

The ability to actively throttle would substantially increase the flexibility of a solid propulsion systems regardless of the mission profile. Fundamental understanding of the micro-scale combustion mechanisms is essential to the development of the next generation technologies for extreme control of the propellant thrust and control by combustion instabilities. Both experiments and theory confirm that the micro- and nano- scale oscillatory networks excitation in the solid propellants reactionary zones is a rather universal phenomenon. In accordance with our new concept, the micro- and nano- scale structures form both the fractal and self-organized wave patterns in the energetic materials (EM) reactionary zones. In particular for each exact frequency of the oscillatory process in the reactionary zone corresponds the unique self-organized spacial patterns of the micro- and nano- scale structures. A novel strategy for smart real-time control of the thrust and combustion instabilities in solid propulsion systems are based on control by self-organization of the micro- and nano- scale oscillatory networks and self-organized patterns formation in the reactionary zones with use of the system of acoustic and electro-magnetic fields, generated by special kind of the electric discharges along with resonance laser radiation. The electric discharges also are capable for excitation of the wave patterns in the reactionary zones. Application of special kind of the electric discharges demands the minimum expenses of energy and opens prospects for almost inertial-free control by combustion processes. Such method of control can be organized with assistance of the neural network-based system. Neural network-based system allows to process, analyze and use the cymatics information - a set of image, acoustic, electro-magnetic and thermal hologrammes that are registered online in the EM reactionary zones. Through online retraining, the neural network-based system can provide precise optimization of the intra-chamber processes and thrust by accommodating of the reactionary zones self-organizing due to flight program and improving operating flexibility. The main advantages of the proposed approach consisted in the natural ability of neural networks in modeling nonlinear dynamics in a fast and simple way and in the possibility to address the process to be modeled as an input-output black box, with little or no mathematical information on the system. The suggested strategy opens new possibilities for enhanced operational capabilities of the next-generation solid propulsion systems.

Detonation in PBX based on RDX – prediction properties and experimental measurements in a divergent detonation propagation configuration

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Keywords: PBX; divergent detonation; detonation wave; THOR code.

The advanced research of Shock (SW) and Detonation Waves (DW) in Energetic Materials (EM) start with prediction properties based in thermodynamic codes. THOR is a program for the prediction of combustion and detonation processes of energetic mixtures. It has been updated during the last 15 years. This code assumes the thermodynamic equilibria for all the possible compounds, including condensed and intermediary species. It can predict Hugoniot and Crussard curves, including the Chapman-Jouguet (CJ) detonation point. JWL constants can then be calculated, assuming the adiabatic or the isentropic expansion of detonation products. It requires a large database (THOR DATABASE) that contains the thermo-chemical properties of the reactants and possible products of reaction. An applied particular case is presented for PBX, based in RDX compositions. However, these thermodynamic predictions do not clarify the phenomenological behavior of the DW propagation. Experimental studies of EM detonation and shock propagations, using optical metrology methods, allow, not only the minimization of testing sample, but also the observation of transition properties of DW propagation. Progress in development of the multi fiber optical probe (MFOP) is presented, discussed, reviewed and systematized, coupled with multiple configuration tests. A particular case is presented: the divergent detonation wave in PBX, in a hemispheric explosive sample, initiated by a long cylindrical charge of the same explosive. The tested PBX is composed by 85 % (in mass) of RDX (bimodal particle distribution, 75 % of d50 = 96um and 25 % of d50 = 22um) and 15 % of binder based on HTPB. This PBX-RDX is presenting an effective density of 1.57 g/cm3, (> 99 % TMD) and detonation velocity of 7.90 mm/μs.The measurements of the pressure of a shock wave, induced not only by the divergent detonation wave, but also by the positive constant curvature detonation wave (detonation in a long cylindrical PBX charge) in an inert standard barrier, show the existence of significant differences, which can reach values up to 2.8 times less, in their amplitudes. Presented experimental results are discussed and correlated with previous model predictions.

Thermal safety predictions for kilo-scales TKX-50 single explosive in storage

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Keywords: TKX-50; thermal safety prediction; finite element analysis; storage of energetic materials.

Dihydroxylammonium 5, 5'-Bistetrazole-1, 1'-diolate (TKX-50) has been widely studied in recent days. However, as a new kind of energetic materials, in addition to its basic properties, researchers are also concerned about its potentially dangerous caused by fire and explosion in production, transportation and storage. In this paper, a improved thermal analysis program was employed for predicting the thermal safety of kilo-scales TKX-50. The running principle of the advanced program is based on a differential isoconversional method, which can be used to obtain the kinetic results and simulation results by employing the data of accelerating rate calorimeter (ARC) and differential scanning calorimetry (DSC). Then, two important safety parameters (time to maximum rate under adiabatic conditions (TMRad) and self-accelerating decomposition temperature (SADT)) for different kilo-scales TKX-50 were obtained and discussed. Finally, the effects of ambient temperature on the thermal explosion of kilo-scales TKX-50 were investigated by using finite element analysis (FEA). The information gained is useful for the storage of kilo-scale TKX-50 in storage, what's more, the method has significant reference value for thermal safety evaluation of other energetic materials during their storages.

Issues related with impurities in binder ingredients of polymer bonded explosive

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Keywords: PBX; impurity; charge quality; sensitivity; compatibility.

In order to describe the influences of impurities in prepolymer and plasticizer on the compatibility, mechanical sensitivities and other properties of polymer bonded explosives (PBXs), two treatment methods were proposed to obtain different purity binder ingredients, viz., convection oven and high temperature vacuum rotary evaporation. Moisture, acidity and purity of raw binders and ingredients after treatment were characterized. PBXs were prepared using both raw and processed binder ingredients. The properties and performance of PBXs were tested respectively. Defective charge quality was found in the PBX using high moisture binder and high mechanical sensitivities were induced by low purity. The results also show that the bulk density and velocity of detonation were changed depending on the charge quality.

Explosive properties of fuel/oxidizer mixtures

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Keywords: fuel/oxidizer; explosives; aluminium; detonation velocity; pressure.

As seen in multiple cases, including the 2013 Boston Marathon bombing, improvised explosives compositions may be as simple as a fuel/oxidizer (FOX) mixture initiated by an electrically-heated wire. The predictive knowledge of large scale explosive potential of fuel/oxidizer (FOX) mixtures is incomplete. Predicting explosive potential from small scale test data is desirable. Herein the explosive properties of fuel/oxidizer mixtures (FOX) were measured at both the small scale (2 g) with bomb calorimetry and large scale (5 kg) with high speed photography and blast pressure probe. Properties measured at the small scale such as the heat and pressure history of closed-vessel reaction were compared to detonation velocity and air blast TNT equivalences measured at the large scale and predictions by Cheetah thermochemical code.

Energetic – Energetic cocrystallization of PETN and RDX

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Keywords: co-crystallisation; performace.

Cocrystallization technique is considered to be one of the most adopted crystal engineering techniques to remove crystal defects which lead to improved material performance. PETN and RDX are secondary explosives which have ester and amine functional groups respectively. Semtex, a commercially available High Energy Material (HEM) made by the physical mixture of PETN and RDX. Cocrystallization technique is proved to yield better crystals possessing high mechanical stability towards friction and impulse, devoid of crystal defects and high chemical homogeneity than physical mixtures. Here we report the cocrystallization of PETN and RDX though ultrasound assisted solvent evaporation technique. The cocrystal obtained further is termed as PRCC. PRCC is further characterized for its structure, morphology and thermal stability employing PXRD, FTIR, FE-SEM and thermal studies (TGA/DTA). Mechanical sensitivity tests such as friction and impact sensitivity, lead block and lead plate acceleration tests, shock tube Velocity of Detonation (VOD) are also used to understand the enhanced performance of as-synthesized PRCC.

Computational studies of the novel tetrazole addition reactions

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Keywords: quantum chemistry calculation; enthalpy of formation; tetrazole; Gibbs free energy; novel high-energetic material.

For the determination of the novel tetrazole and N-dimethylmethanamine addition reaction mechanism the quantum-chemical calculations (DFT B3LYP) have been done. The Gibbs free energies of starting compounds, products (intermediates) and transition states in addition reaction have been estimated. It is shown that tetrazole is very stable to proton separation, but easily reacts with N-dimethylmethanamine in the set of reactions.ere. Use about 300 words.

Experimental investigations on rheological properties and viscoelastic constitutive model verification of pasty propellant

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Keywords: pasty propellant; rheological property; experimental investigation; constitutive model.

The rheological properties of the pasty propellant were studied by using a rotary rheometer. Based on the creep test results of the pasty propellant, a three-parameter viscoelastic constitutive model of the patsy propellant was established and verified. The change of the strain with time can be divided into two stages. When the time is less than 50 seconds, the strain of the pasty propellant is influenced by the elastic effect and it changes nonlinearly with time, and when the time is greater than 50 seconds, it shows that the effect of the elastic effect smaller and the strain changes linearly with time. At the same time, the relationship between the shear stress and viscosity of the propellant with shear rate and temperature were investigated. The results show that the shear stress of the pasty propellant increases with the increase of the shear rate, and the viscosity decreases with the increase of the shear rate. The power law model can be used to describe the relationship between the viscosity and shear rate of the pasty propellant; for the influence of temperature, the viscosity of the pasty propellant decreases when temperature increases and which satisfies the Arrhenius relationship, all parameters in the correlation formula are obtained according to the experimental results.

Preliminary analysis of usage prospects of nitrogen-rich energetic heterocycles

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Keywords: enthalpy of formation; density; chemical structure; explosive characteristics.

The analysis of the chemical structure characteristics, their interrelations with the enthalpy of formation and the monocrystal density is executed with the usage of statistical methods on the basis of the database including more than 1000 solid organic substances, atoms containing carbon, hydrogen, oxygen, nitrogen, sulfur and fluorine. MAS method is developed on the basis of the additive approach, allowing to carry out estimation of the enthalpy of formation and the monocrystal density on the basis of the corresponding contributions of the atoms making a molecule, into the property. The efficiency of the method is illustrated by the example of calculations of the parameters of compounds of various chemical classes. For a series of the derivatives of tetrazole, oxadiazole and tetrazine, physical and chemical parameters are calculated and prospects of their usage as high energy density substances are estimated.

Effect of vertical concentration gradient on globally planar detonation with detailed reaction mechanism

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Keywords: detailed reaction; WENO; additive Runge-Kutta (ARK); concentration gradient.

Since detonation often initiates and propagates in the non-homogeneous mixtures, investigating its behavior in non-uniform mixtures is significant not only for the industrial explosion in the leakage combustible gas, but also for the experimental investigations with a vertical concentration gradient caused by the difference in the molecular weight of gas mixture. Objective of this work is to show the detonation behavior in the mixture with different concentration gradients with detailed chemical reaction mechanism. A globally planar detonation in H_2-O_2 system is simulated by a high-resolution code based on the fifth-order weighted essentially non-oscillatory (WENO) scheme in spatial discretization and the third-order Additive Runge-Kutta schemes in time discretization. The different shocked combustion modes appear in the rich-fuel and poor-fuel layers due to the concentration gradient effect. Globally, for the cases with the lower gradient detonation can be sustained in a way of the alternation of the multi-heads mode and single-head mode, whereas for the cases with the higher gradient detonation propagates with asingle-head mode.

Sensitivity evolution of NEPE propellant during ageing

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Keywords: NEPE propellant; ageing; fuzzy comprehensive evaluation; safety.

With high level of output energy, NEPE (Nitrate Ester Plasticized Polyether) propel-lant has attracted considerable attention. However, it also suffers from ageing prob-lems due to the decomposition of the nitrate ester plasticizer and production of NO_2, which results in further decomposition of polymer substrate. Besides aroused me-chanical problems, this process can also lead to a safety problem. To investigate the sensitivity evolution of NEPE propellant during storage life, varia-tions of 5-second explosion temperature, volume of released gas in vacuum stable test, characteristic drop height, 50% explosion pressure and static spark energy with accelerated ageing time were monitored and the results were treated with fuzzy com-prehensive evaluation (FCE) method. A tendency of increasing sensitivity was noticed. The results show that after approximately 36 45 days' ageing under 70 ºC, the sensi-tivity went through a step change. The pores created by the integrity compromise of polymer structure during ageing accounts for the sensitivity evolution of NEPE pro-pellant. As such, the discovery of more effective stabilizer is urged to improve the storage safety of NEPE propellant.

Analysis of non-ideal detonation behaviour based on analog system

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Keywords: analog system; detonation; criticality ; instability.

The paper builds the analog system of detonation with loss and the chemical reaction of two step reaction model, wherein an induction zone is followed by a energy and heat release zone. Steady state of detonation wave structures are obtained by analytic method. By changing the value of the sensitivity exponent of reaction rate n and the sensitivity coefficient of loss rate m, we can get the diagrams of steady detonation velocity and the loss coefficient κ under the corresponding parameter and detonation failure of linear boundary, and derive the critical characteristics of detonation failure conditions finally. In view of the above established the analog system of detonation, through the linear stability of the normal mode analysis, it is clear to deduce the spreading condition by means of limiting the spread of the disturbance to the upstream, study the stability of the steady state solution under the condition of the ideal and non-ideal (with loss) analog system of detonation and the influence of related parameters on the stability.

Thermal hazard assessment of TKX-50 under adiabatic condition

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Keywords: TKX-50; hazard assessment; accelerating rate calorimeter; SADT.

The hazard assessment of TKX-50 was studied under adiabatic condition by using acceler-ating rate calorimeter (ARC). RDX, HMX and CL-20 were also studied to compared with TKX-50. The adia-batic experiment obtained the data include initial self-heat temperature, adiabatic temperature rise and temperature rise rate, etc. The data of adiabatic decomposi-tion kinetics and the value of SADT were calculated. The results show that the adiabatic in-itial self-heat temperature of the four explosives are all above 180°C. The maximum tem-perature rise rate of TKX-50 is the lowest in the four explosives, which indicate the decom-position process of TKX-50 is the mildest. Assessing the thermal safety by SADT is in the order of HMX>TKX-50>CL-20>RDX.

High-nitrogen 1D energetic complexes based on novel C-N linked 2, 5-ditetrazolyl-1, 3, 4-triazole (DTT)

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Keywords: coordination compounds; 2,5-ditetrazolyl-1,3,4-triazole; high nitrogen.

Herein we synthesized two new one-dimensional high-nitrogen coordination compounds DTTK and DTTNa by using C-N linked 2, 5-ditetrazolyl-1, 3, 4-triazole (DTT) as a ligand. All new energetic compounds were fully characterized by IR and elemental analysis, and DTTK and DTTNa were further determined by single-crystal X-ray diffraction analysis. DTT is a new compound with a novel structure and high nitrogen content (76%), which is more than those of commonly used high energetic explosives. DTTK and DTTNa have high energetic positive heats of formation (DTTK: 614.8 $kJ \cdot mol^{-1}$; DTTNa: 689.8 $kJ \cdot mol^{-1}$) and good energetic properties. (DTTK: D = 7.546 $km \cdot s^{-1}$, P = 20.7 GPa; DTTNa: D = 7.962 $km \cdot s^{-1}$, P = 23.2 GPa).

Effect of hydrophobicity of FOX-7 particles on rheological properties of slurry and compressive strength of PBX

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Keywords: FOX-7; PBX; hydrophobicity; wettability.

The hydrophobicity of particles have significant impact on the process performance and mechanical characteristics of many kinds of particle-filled polymer composites. Therefore the hydrophobicity of energetic particles would have great effect not only on the rheological properties and process performance of slurry but also on the final qualities of PBX products. In this study, the rheological properties of slurry and compressive strength of PBX filled with pristine FOX-7 particles and particles after hydrophobic treatment with hexadecyltrimethoxysilane were compared. The static contact angle of FOX-7 particles with HTPB and water increased significantly after hydrophobic treatment. As a result,the increase of loss factor indicated that the slurry filled with hydrophobic FOX-7 particles exhibited a better leveling performance. The results suggested that the wettability of particle surface is one of the key factors that determined density and compressive strength of PBX products. Furthermore, the mixture of pristine FOX-7 particles and hydrophobic particles showed a middle status of wettability. Herein it might be considered as a promising method to regulate rheological properties of PBX slurry and further to ameliorate the leveling perfomance.

Effect of boron coated with AP on the underwater explosion performance of RDX-based explosives

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Keywords: boron coated with AP; underwater explosion.

In order to study the Born coated with AP on the performance and reaction behavior of underwater explosives,a series of underwater explosion (UNDEX) tests that used a 1kg cylindrical charge was conducted underwater at a depth of 8m.The pressure histories of the shock wave produced at different positions and the bubble periods were measured.Based on the experimental results of the shock wave,the coefficients of similarity law equation for the peak pressure and attenuation time constant of shock wave were in acceptable agreement.The result show that,underwater effective total energy of RDX/(AP-B)-based explosives was higher than RDX/B-based explosives.

Theoretical investigation on the structure and energetic performance of new high-energy nitramine explosives

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Keywords: high-energy-density material; nitramine; explosive; energetic properties.

Carefully analyzing the structural traits of well-known explosives, RDX (1,3,5-trinitroperhydro-1,3,5-triazine) and HMX (Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine), a series of nitramines with –CH2NNO2– structural unit was designed and studied using the B3LYP/6-31G* method within the density functional theory (DFT). The diverse geometries are ranging from linear (Model IA and IB) to cyclic (Model II) to caged (Model IIIA and IIIB) structures. Computational results show that the energetic parameters, i.e., density (p), detonation velocity (D), and detonation pressure (P), decrease in the order of IIIBn > IIIAn > IIn > IAn > IBn with the same number of the –CH2NNO2– unit (n). The contribution of each additional –CH2NNO2– to density per unit (r/n) decreases gradually, which results in the energetic properties of linear nitramines increase first and then keep stable with the increasing n. This effect clearly indicates that elongating the chain length infinitely (e.g., polymerization) brings very little benefit in boosting the explosive properties. Promisingly, all compounds in Models IIIA and IIIB have achieved better or comparable energetic properties than the benchmark explosives, RDX, HMX and CL-20 (2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane). Consideration on the reality, synthesis of molecules of IIIAn and IIIBn (n = 1−3) will most likely bring a new generation of super-powerful explosives to the market.

Desensitization and stabilization mechanisms of graphene on energetic transition metal complexes

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Keywords: graphene oxide; metal complexes; thermal stability; activation energy.

The graphene oxide (GO) was found to be able to stabilize organic molecules including energetic compounds. However, the stabilization effect and inherent mechanisms are still not well known. It has been shown that the presence of GO could great improve the thermal stability of the TAG-Ni complex with the peak temperature increase of more 13 °C. The GO decomposes with peak temper-ature of 223.2 °C with heat release of 1063.6 J g-1 at a heating rate of 5 °C min-1, and its decompo-sition activation energy of GO is about 161.3 kJ mol-1. The initial heat release process of GO follow phase boundary controlled reaction model (R2), but its mass loss process matches well with two-dimensional diffusion model (D2). The initial step mass loss of GO was caused by loss of physically bond water molecules, while there are also H2O and a large amount of CO2 and CO produced later on. The GO would greatly decrease the activation energy (Ea) of TAG-Ni from 129.2 to 75.1 kJ mol-1. The reaction model for heat flow of G-T-Ni decomposition is close to the D2 model, whereas its mass loss process follows a random two-dimensional nucleation and nucleus growth model (A2).

Microwave methods to measure the burning rate of energetic materials

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Keywords: microwave methods; burning rate; measurement; energetic material.

Starting from 1960s the microwave methods with the microwave wavelengths 30, 8 and 2 mm are effectively used for measuring the burning rate of energetic materials (EM). Classical option of the microwave method is based on registration of the data in the form of interferogram. When measuring the phase difference between the reference signal and the test signal passing through the sample under study (energy supply from the cold end), the resulting signal has a sine form with amplitude depending on the attenuation of the microwave radiation inside the EM. As an advanced option it can be proposed method based on use of quadrature detector in order to record simultaneously the sine and cosine components of the resulting signal. In this case the rate of the signal phase variation determines instantaneous regression rate of the propellant. The above options are applied typically for measuring the burning rate of solid samples of EM. For the EM samples with internal channel the novel microwave resonator technique was recently developed, which allows measuring the current mass of sample with the high parameters of mass and time resolution. When working with microwave meters, one should take into account several factors reducing the data accuracy. These are Vibration of Experimental Setup, Compressibility of EM, Reflection from the Flame Plasma, Variation in the Dielectric Properties of EM, Burning-Surface Roughness, and Instability of Performance Characteristics of Recording Devices. Correct interpretation of experimental data takes careful analysis of the effects of listed factors. However, it can be noted that the microwave methods have potentially the best characteristics in terms of time and pace resolution among existing experimental methods.

Experimental studies on vertical detonation characteristic of strip-shaped transfer charge

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Keywords: explosive train; strip-shaped transfer charge; shock wave attenuation; detonation transfer.

In order to determine the thresholds and detonated path of the strip-shaped transfer charge used in the flatbed explosive train, an explosive train sample using JO-9C(III) strip-shaped transfer charge was designed to study the minimum thickness of thestrip-shaped transfer charge and the minimum safe distance between transfer charge and the electric detonator. The transfer experiments were conducted using explosive train of dif-ferent thick strip-shaped transfer charge in which the electric detonators were in an armed position. The detonation interruption experiments were followed conducted using explosive train with different safe distances. The shock wave attenuation rule is applied to verify the experimental results and determine the detonated path. The calculated and experimental results were in very good agreement. The results show that the minimum thickness ranged from 0.2mm to 0.4mm, the minimum safe separation distance ranged from 0.4mm to 0.6mm; and the strip-shaped transfer charge is detonated by a shock wave from rather than air clearance when the safe distance is less than the minimum threshold.

Synthesis of nitrocompounds in compressed Freon medium

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Keywords: nitration; nitramine; nitro ester; dinitrogen pentoxide; 1,1,1,2-tetrafluoroethane.

For the first time liquefied 1,1,1,2-tetrafluoroethane (TFE) has been successfully applied as the reaction medium for safe and sustainable synthesis of various nitro esters and N-nitro products via nitration of corresponding alcohols and amides with dinitrogen pentoxide. Freon's inertness towards both electrophilic and nucleophilic agents allowed for a convenient one-pot approach to N-nitramines that comprised nitration of N,N'-dialkyloxalamides or N-alkylcarbamates with N_2O_5 followed by ammonolysis of obtained N-nitroamides in the same fluid solvent without any intermediates isolation. The proposed methods are attractive due to the significant advantages they offer, i.e. high yields, environmental benign, mild reaction conditions, low operation pressure, and facile solvent recycling.

Bioinspired polydopamine coating on the surfaces of energetic materials to enhance the interfacial mechanical performances

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Keywords: polydopamine coating; tatb@pda; interfacial film; adhesive properties; mechanical performances.

The materials coated with the robust and integrated film, combined with excellent wettability and high interfacial mechanical strength are important for the development of composite materials. Inspired by the foot protein of mussels, the energetic material TATB coated with the self-assembling polydopamine were prepared by a simple solution stirring process in the study. Because of the roughness constructed by nanoscale structures and the higher surface energy for the coatings, the as-prepared TATB@PDA showed better wettable properties by water and thermosetting resin compared with the original TATB. The excellent wettabilty could improve the adhesive property between the TATB@PDA and resin in the slurry. Furthermore, the mechanical performances of the grains for TATB@PDA-resin were better than that of the grains for TATB-resin, which were due to the excellent wettability, enhanced adhesive properties and riched active groups for the surfaces. The results of this study might provide the bioinspired polydopamine coating as a superior interfacial film to enhance the adhesive and mechanical performances used in composite materials.

Numerical simulations and field validation tests for shock waves propagation

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Keywords: numerical simulation; field-test; shock wave; Friedlander curve.

At the BAM test range in Horstwalde a number of field trials were conducted with a HE to investigate the free field propagation of shock waves and that resulting from reflection at structure surfaces. In addition, the behavior of the structure under the effect of the dynamic pressure waves after explosion was studied. For both the tests, (a) with a 30 cm thick reinforced-concrete wall and (b) in free field, pressure was measured over the entire test duration with piezoelectric sensors at distances of 5, 10 and 15 m from the detonation center for a range of HE quantities. Apart from this, high speed footage of the tests was recorded as well. Corresponding to the field tests, numerical simulations of HE detonation were performed using APOLLO BLASTSIMULATOR, a CFD tool developed by Fraunhofer Institute for High-Speed Dynamics, Ernst-Mach-Institute. The accuracy of the simulation results as well as the computing times depend on the spatial grid resolution. The outputs of grid-independence study demonstrated that the peak pressure is higher and the pressure-rise is steeper for simulation runs with a finer grid. Remarkably however, the exponential pressure decline is independent of the grid resolution. Advantage was taken of this feature to obtain improved peak pressure values from comparatively coarser grids, in that curve-fitting was performed using the Friedlander Equation, which is well documented in literature. The simulation results for pressure-time histories were compared with the field-test results at the corresponding measurement positions. The two data sets showed good correlation in case of scaled distances greater than 5 [m $kg^{-1/3}$] for both peak pressure and impulse values. This conclusion could be drawn for both trial-types: free-field and with reflection wall. The near field region, on the other hand, necessitates further investigation for the validation of numerical simulation.

Reaction of S,S'-dimethyl-N-nitroimidodithiocarbonate with 5-aminotetrazole

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Keywords: S,S'-dimethyl-N-nitroimidodithiocarbonate; 5-aminotetrazole; 2-methyl-1-nitro-3-(tetrazol-5-yl)-isothiourea; 1-(tetrazol-5-yl)-2-nitroguanidine.

Reaction of S,S'-dimethyl-N-nitroimidodithiocarbonate with 5-aminotetrazole and its potassium salt has been investigated. The product of the reaction of nucleophilic monosubstitution is 2-methyl-1-nitro-3-(tetrazol-5-yl)-isothiourea. The resulting compound has been studied by mass spectrometry and elemental analysis, as well as studied by NMR, FTIR and UV spectroscopy. The presence in the molecule of the methylthio group –SCH3, which can go away with the subsequent nucleophilic substitution, makes it possible to use it as a precursor for the synthesis of energetic derivatives of 1-(tetrazol-5-yl)-2-nitroguanidine.

Characterization of HNIW precursor TADBIW, synthesized via HBIW

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Keywords: HNIW; TADBIW; HBIW.

HNIW is promising explosive and in recent years there are various attempts for low cost, low toxic, high yield, high purity synthesis methods with different precursors. HNIW requires multi-step synthesis and cage structure is created at first step as HBIW and in many different synthesis routes, the next step is debenzylation of HBIW to TADBIW. So, to reach HNIW with different routes, TADBIW is a key step to investigate. In the past studies most of the characterization effort focused on the final product but the intermediates or precursors still needs more attention. In addition impurities in final product HNIW, affect negatively the impact and/or friction sensitivities, so determination of purity levels of the precursors in various routes become an important point. In this study TADBIW that is synthesized via HBIW and characterized by HLPC, prep-HPLC, LC-TOF, NMR, PVM, MasterSizer, density, BET, FTIR, TGA-DSC.

Combustion temperature measurement of calcium sulfate dihydrate/aluminium thermite mixture

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Keywords: thermite; combustion; calcium sulfate dihydrate; aluminium; FLIR.

Calcium sulfate dihydrate is used as an oxidizer for thermite mixtures with micron sized aluminium powder. Samples were ignited using boron-potassium nitrate mix-ture and the combustion temperature measurement was carried out by using an in-dium antimonide (InSb) focal plane array cooled infrared camera (FLIR mod. SC 7200) working in camera the mid-IR spectral range and using a pyrometer Two-Colour-High-Speed-Pyrometer Metis H311 (Sensotherm GmbH).

Kinetic model of explosive gas formation in condensed systems

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Keywords: condensed state; metastability; steam explosion; stationary states manifold; detailed equilibrium; turning point.

In nature and technology, there are phenomena when fast explosive changes in thermodynamic parameters occur in chemically neutral systems, exchanging energy with the environment. Examples are explosions of autoclaves, magmatic foci of volcanoes, meteorites in the atmosphere. The causes of such phenomena have long been discussed in the literature, but until now they have not found an established theory. One possible way of explaining is to consider at an elementary stage level the nonisothermal kinetics of the process of evaporation of a condensed substance in a homogeneous closed system of particles containing a condensed and a gas phase under conditions of supply of an energy flux. This mathematical model naturally describes jumps in the gas components and it pressure in the establishment of detailed equilibrium and the transition through metastable states. The application of the model to the two-component water-vapor system showed that it reproduces the observed series of explosions of the Chelyabinsk meteorite in a qualitatively correct manner.

Vapor pressure measurements of melt cast explosives with gas-saturation method

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Keywords: vapor pressure; melt cast.

This work is focused on measurements of the vapor pressure of melt cast explosives DNAN and TNT with the gas-saturation method. A carrier gas stream is saturated with the analyte of choice at a well-defined temperature and flow-rate. Subsequently the analyte is resublimed in a cooling trap and quantified by GC-MS or HPLC analytical systems. The vapor pressure, enthalpy of sublimation and other physico-chemical data can be calculated from the experimental results. Literature-unknown vapor pressure values of energetic materials were determined. These results of this work are be of a great value for the detection of explosives.

Influence of charge diameter on detonation velocity for single and double base propellants

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Keywords: detonation velocity; charge diameter; propellant; nitrocellulose.

Charge diameter has very significant influence on detonation parameters. Detonation performance of nitrocellulose based propellants was investigated. Cylindrical charges with grains of different domestically produced single and double base propellants were considered. Detonation velocities were experimentally determined for these charges with different charge diameter and initial density. Experimental results were analysed using the methods of regression analysis in order to determine critical diameter and parameters of charge diameter influence on detonation velocity.

Comparison of burning rate modifiers on the example of a composite rocket propellants based on sodium nitrate

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Keywords: composite propellant; HTPB; sodium nitrate; burning rate.

This paper presents the results of the comparison of three widely used burning rate modifiers on the example of composite rocket propellants based on sodium nitrate. A series of composite rocket propellants with 1% additive of the catocene, copper chromite and nanoiron oxide were prepared and tested. For each propellant, such parameters as caloriffic value, hardness, sensitivity to mechanical stimuli and pot-life were determinated. The ballistic parameters of the investigated propellants were determined by combustion in a laboratory rocket motor (LRM).

Following isocyanate-polyol curing by volume shrinkage induced pressure decrease – considering reaction volume, activation volume, compressibility and diffusion control

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Keywords: polyol-isocyanate curing; modelling of curing; volume shrinkage by curing; pressure dependence of rate constant; bulk compression modulus; diffusion control during curing.

To know the completion of the curing reactions used to create elastomers is an important aspect in controlling the curing process and in considering the ageing of the elastomer. The so-called post-curing must be separated from real ageing. The reaction kinetic description of curing reactions gives activation parameters and heat of reactions with thermal methods. The tracking of curing reaction via volume shrinkage is an interesting aspect because normally calorimetric methods cannot be applied with real systems. To use the volume shrinkage is possible in a constant volume device, filled up with the reaction mixture and held under a certain overpressure during the monitoring. By the curing, the reaction mixture shrinks, and the pressure drops. By this, the kinetic analysis is possible. At this point, one has to consider pressure influence on the reaction rate constant and the change of bulk compressibility or the compression modulus with the increasing degree of curing, means cross-linking. It is reasonable to assume that the uncured reaction mixture has a lower isothermal compression modulus than the cured mix. This paper gives the analyses of the pressure influence on the reaction rate constant in connection with the reaction kinetic description and the effect of change of compression modulus on the kinetic evaluation via pressure decrease. A further topic with curing reactions is the diffusion control during the later curing process. A solution is offered, which works with any probing method, number of species, thermal or volume shrinkage.

Reactions of dinitropyrazoles

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Keywords: explosive; pyrazole; nitrogen-rich; sensitivity; crystal structure.

The synthesis of 3,4- and 3,5-dinitropyrazole derivatives is described. Nitrogen-rich salts of the two different isomers were synthesized by metathesis reaction in order to tune performance and sensitivity values. Further, two different bridged dinitropyrazoles were obtained to increase the oxygen balance as well as the thermal stability. The obtained compounds were characterized using low temperature single crystal X-ray diffraction, vibrational (IR, Raman) spectroscopy, multinuclear NMR spectroscopy, mass spectrometry, elemental analysis and DSC measurements. The sensitivities toward external stimuli (impact, friction and electrostatic discharge) were determined according to Bundesamt für Materialforschung (BAM) standard methods. The energetic performances were calculated using the EXPLO5 code and support the high energetic character of the title compounds. Heats of formation were computed by the atomization method based on CBS-4M electronic enthalpies.

Application of rapid screening device test to evaluate the thermal stability of gun propellant

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Keywords: kinetic parameter; gun propellant; thermal stability; RSD; DSC.

Rapid Screening Device (RSD) has never been employed to determine thermal decomposition kinetics of energetic materials. In this paper, the thermal degradation energy (Ea) of two simple base gun propellants was investigated. One of the investigated propellants is naturally older than the second but both have similar chemical composition. The value of the activation energy was evaluated by applying Kissinger's method from RSD results. Assessing the thermal decomposition kinetics of propellants by RSD tests is an added value to the range of thermal analysis tests if the results of these tests can be well correlated to the results of existing thermal analysis technique. Therefore, a comparison was made and the decomposition energies of both investigated propellants were determined isothermally by ignition delay technique and non-isothermally by DSC test. A correspondence has been observed between all the thermal analysis methods employed in this study. In fact, RSD, ignition delay technique and DSC results show that the older investigated propellant has lower activation energy.

Problems of granulation of energetic compositions based on nitrocellulose

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Keywords: energetic material; pyrotechnic; solution; granulation; nitrocellulose.

The production of some energetic materials is associated with process of its granulation. In the case of compositions containing nitrocellulose, established their high sensitivity to process parameters. This fact was a prerequisite for conducting studies to determine dependence the viability of nitrocellulose varnish on the quality of the granulated product.

A fast and feasible synthesis for picryl bromide

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Keywords: picryl bromide; 2-bromo-1,3,5-trinitrobenzene; synthesis; energetic material.

A new and optimized procedure for the synthesis of picryl bromide is described. A previous procedure involved a two-step nitration of bromobenzene, using a nitration mixture consisting of concentrated sulfuric acid and white-fuming nitric acid for 17 and 12 hours at 140 °C. The crude product obtained in this way is then submitted to two subsequent crystal transformations from boiling ethanol, which makes this procedure very time-consuming. A second previous procedure used a nitration mixture consisting of concentrated sulfuric acid and potassium nitrate at 125 °C for 6 hours to achieve the direct one-step nitration of bromobenzene with yields of up to 60%. A third procedure used 1,3,5-trinitroanisole as the starting material, which was submitted to a two-step bromo-demethoxylation reaction, using KI/EtOH and PBr3 as the key reagents to obtain the target compound. The key problem with this route of synthesis is the availability and price of the starting material. The newly disclosed procedure involves the direct one-step nitration of bromobenzene using a 5:1 mixed acid, consisting of oleum (30%) and white-fuming nitric acid (10 equivalents), as the nitration agent. The reaction mixture is stirred for 45 minutes at 0 °C and then heated to 130 °C using an aluminum heat block. It is kept at that temperature for 3 hours and afterward cooled to room-temperature. The mixture is then poured into ice-water and washed with large amounts of cold water to obtain up to 63% picryl bromide in pure form without crystal transformation or further purification. This method combines the use of cheap materials with a time-economic route of synthesis and less to no additional purification steps, which is an improvement compared to the state of the art methods.

Study of sesitivity to impact for explosive mixes HMX with metallized components

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Keywords: impact; explosion; sensitivity; sensitizing.

In experiments on sensitivity quantitative estimation to impact by tensometric method of critical pressure for mixes Oktogen with Ferric oxide (Hematite) of various composition is detected the phenomenon of a strong sensitisation of the mix which sensitivity in a point of a minimum of an indicator of critical pressure of explosion initiation is on the level of high-sensitivity explosive PETN. And hypersensibility of a mix is fixed in a wide range of oxide maintenances from 20 to 60 % (weights). The mathematical model of explosion initiation of the mix, based on conception about ignition Oktogen by frictional heated up particles of oxide during the moment of mechanical failure of mixed charge at impact is offered.

Determination of amine residues after explosion

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Keywords: HPLC; amine.

A simple and sensitive method for the determination of free aliphatic and aromatic amines using derivatives agents (dansyl chloride, 9-fluorenylmethyl chloroformate and 4-Chloro-7-nitrobenzofurazan) as a labelling reagent by high-performance liquid chromatography with fluorescence detection (HPLC-FLD) has been developed. Derivatization conditions including reagent concentration, buffer pH, reaction time and temperature were optimized. A fluorescence derivatization - high-performance liquid chromatography (HPLC) method, which enables the femtomole-level detection of analytes, is a powerful tool for the analysis with high sensitivity and selectivity. In recent decades, improvised explosive devices (IEDs) have become an increasing topic of public concern, with high-profile incidents such as the Bali (2002), London transport (2005), Boston Marathon (2013) and Brussels (2016) bombings garnering mass international attention. Although the majority of media coverage has focused on large-scale incidents, there has also been a rise in explosive incidents involving smaller devices such as pipe bombs. This is particularly the case in the United States, where pipe bombs are considered to make up the vast majority of IED encounter. These devices can be easily constructed from everyday materials. The mixture nitromethane with amines is applicable for this. Determination of residues after an explosion is important. This method (HPLC-FLD) could be useful for their determination. The proposed method is sensitive and reproducible for the determination of aliphatic and aromatic amines.

Effect of particle size on the performance of MTV decoy flare compositions

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Keywords: decoy flares.

Decoy flares provide the main protection to different air fighter against different IR guided missiles working on different bands as (α) (1.8 - 2.5 μm) and mid wave (β) (3.5 - 4.8 μm) band. Different particle size of fuel (Mg) for one selected decoy flare compositions is the main content of this paper. Sample (1) with particle size (63μm), sample (2) with particle size (150 μm), and sample (3) with particle size (200 μm) have been tested Experimental evaluation for different particle size was carried out by measuring flame temperature and burning time using in Fra metric radiometer. Radiant emittance was calculated using designed computer program. Results show that, sample (3) with particle size (200 μm) has highest radiant emittance and sample (1) with particle size (63μm) has longer burning time so the particle size would be predetermine precisely when designing decoy flare compositions.

Effect of pressing force on the performance of MTV flare compositions

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Keywords: pyrotechnic; decoy flare.

Pyrotechnic decoy flares are represent the most effective tools for countering against IR guided missiles. The developments on the IR seeker make the researcher to studying different parameter that affect the performance of different kinds of decoy flares. Also different operating conditions when using decoy flares are very important for studying. Pressing force represent one of the processing parameter that affect burning time, flame temperature, and radiant emittance. In this study, different applied pressing forces ranging from (0.5 to 1.5 KN) are experimentally tested for selected MTV compositions. Burning time, flame temperature, and radiant emittance have been measured using IR radiometer and the density changes also recorded. The result shows that 0.5 KN is the optimum for using on MTV decoy flare compositions

Solid-state extrusion of energetic materials

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Keywords: energetic material; pyrotechnic; extrusion; high density; polymer.

Extrusion is widely used in the processing of energetic materials as the most productive technology. In the traditional meaning, extrusion is the technology of obtaining products by forcing a viscous melt of a material or a thick paste through a die. Pyrotechnics is a particular class of energetic materials, which is processing only in the solid-phase state at the temperatures below the melting temperature of the binder component. The paper shows the principal possibility of a solid-phase extrusion of pyrotechnic materials and the influence of this method on their characteristics.

The application of nitrocellulose and ammonium perchlorate granules for solid rocket propellants formed by loading method

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Keywords: nitrocellulose; ammonium perchlorate; energetic plasticizer; CMDB; loading method.

Nitrocellulose granules are used for the production of smokeless powders or solid rocket propellants. The application of nitrocellulose and ammonium perchlorate granules for formation of solid rocket propellants (composite modified double base propellants) using loading method was presented. The influence of energetic plasticizer type (nitroglycerin, N-butylnitroxyethylnitramine, diethylene glycol dinitrate) on properties of propellants was determined. The thermochemical and termodynamical properties were calculated based on the bulk density of mixtures contain nitrocellulose and ammonium perchlorate granules. The propellants' samples were characterized by optical microscope and thermogravimeter. The characterized samples show sufficient thermal stability in terms of the safety of manufacturing process. The dependence of activation energy on conversion degree was divided into three stages and this observation is similar to all obtained propellants' samples. The studies indicate the possibility of using plasticizers N-butylnitroxyethylnitramine and diethylene glycol dinitrate for composite modified double base propellants, which unlike nitroglycerin, have less negative impact on the human body and are less sensitive to external stimuli.

Molecular properties and explosion performance of 5,5'-bis(1H-tetrazolyl)amine and its three derivatives

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Keywords: bistetrazolylamine; derivatives; molecular properties; decomposition mechanisms; detonation parameters; exploding action..

New calculated results were obtained for 5,5'-bis(1H-tetrazolyl)amine and such its derivatives as 5,5'-bis(1H-tetrazolyl)amine monohydrate, 5,5'-bis(2-methyltetrazolyl)amine and 5,5'-bis(2-methyltetrazolyl)methylamine. Quantum chemistry methods implemented in the Gaussian 09 computer program were used first of all. The B3LYP hybrid functional was used and a number of basis sets, from 6-31G(d) to 6-31++G(3df,3pd), were tested in performed calculations. All possible molecular properties of considered explosive substances were determined for isolated molecules. The main primary decomposition mechanisms were determined for all of them. The complexes of several interacting molecules were examined too. The enthalpies of formation of studied substances in the gas phase were calculated using the CBS-4M and CBS-QB3 complete basis set methods in the atomization energy and isodesmic reactions approaches. The Trouton rule and the method of electrostatic potential were chosen for estimations of the enthalpies of sublimation. All parameters of detonation waves and detonation products were determined using the EXPLO5 thermochemical program. Such calculations were performed for different initial densities of explosives. Numerous calculations of exploding action of examined explosives were conducted using the ANSYS Autodyn program. Thick barriers of different materials and copper plates of different thicknesses were used for such calculations. All new calculated results were compared with experimental and calculated results obtained for these substances earlier.

Molecular properties and explosion performance of 5-aminotetrazolium and diaminotetrazolium nitrates

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Keywords: aminotetrazolium nitrate; molecular properties; decomposition mechanisms; detonation parameters; exploding action..

New calculated results were obtained for two explosive nitrates such as 5-aminotetrazolium nitrate and diaminotetrazolium nitrate. Quantum chemistry methods implemented in the Gaussian 09 computer program were used first of all. The B3LYP hybrid functional was used and a number of basis sets, from 6-31+G(d) to 6-31++G(2d,2p), were tested in performed calculations. All possible molecular properties of considered explosive substances were determined for molecular units and ions included in their composition. The main primary decomposition mechanisms were determined for complete molecular units and separate cations. The complexes of several interacting molecular units were examined too. The enthalpies of formation of explosive substances in the gas phase were calculated using the complete basis set (CBS-4M, CBS-QB3, CBS-APNO) and Gaussian-n (G3, G4) methods in the atomization energy approach. The Jenkins model and the method of electrostatic potential were chosen for estimations of the enthalpies of crystal lattices. All parameters of detonation waves and detonation products were determined using the EXPLO5 thermochemical program. Such calculations were performed for different initial densities of explosives. Numerous calculations of exploding action of examined explosives were conducted using the ANSYS Autodyn program. Thick barriers of different materials and copper plates of different thicknesses were used for such calculations. All new calculated results were compared with experimental and calculated results obtained for these explosive substances earlier.

Molecular and detonation properties of hexaamminecobalt(III) and aquapentaamminecobalt(III) perchlorates and hexaamminecobalt(III) nitrate

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Keywords: hexaamminecobalt(III) perchlorate; hexaamminecobalt(III) nitrate; molecular properties; decomposition mechanisms; detonation parameters.

New calculated results were obtained for two amminecobalt(III) perchlorates and one amminecobalt(III) nitrate, which are the basic substances for developing more advanced tetrazolatoamminecobalt(III) explosives. They are hexaamminecobalt(III) perchlorate, aquapentaamminecobalt(III) perchlorate and hexaamminecobalt(III) nitrate. Quantum chemistry methods implemented in the Gaussian 09 computer program were used first of all. The B3LYP hybrid functional was used and several basis sets, from 3-21G to 6-31++G(2d,2p), were tested in performed calculations. All possible molecular properties of considered explosive substances were determined for molecular units and ions included in their composition. The main primary decomposition mechanisms were determined for complete molecular units and separate cations. The enthalpies of formation of the substances in the gas phase were calculated using the complete basis set (CBS-4M, CBS-QB3) and big basis set DFT methods. The Jenkins model was chosen for estimations of the enthalpies of crystal lattices. All parameters of detonation waves and detonation products were determined using the EXPLO5 thermochemical program. Such calculations were performed for different initial densities of explosives. All new calculated results were compared with experimental and calculated results obtained for these substances earlier.

Molecular properties and intermolecular interaction for 1,1-diamino-2,2-dinitroethene and its three cyclic homologs

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Keywords: diaminodinitroethene; cyclic homologs; molecular properties; intermolecular interaction; decomposition mechanisms; clusters.

New calculated results were obtained for 1,1-diamino-2,2-dinitroethene and such its cyclic homologs as 2-(dinitromethylene)-1,3-diazacyclopentane, 2-(dinitromethylene)-1,3-diazacyclohexane and 2-(dinitromethylene)-1,3-diazacycloheptane. Several calculating methods implemented in the Gaussian 09 computer program were used for this purpose. All possible molecular properties of considered explosive substances were determined for isolated molecules. The main primary decomposition mechanisms were determined for all of them. The complexes of interacting molecules up to 5 in size were examined too. The density functional method with the B3LYP hybrid functional and the 6-31+G(d,p) basis set was used for these calculations. Small clusters of up to 30 molecules in size were studied too. Their structure and energetics were calculated using the methods of molecular mechanics and semi-empirical quantum calculations. A rather clear comparative picture was obtained for all the homologous substances examined in terms of the trends in the variation of their molecular properties and the nature of their intermolecular interaction. Some of these new calculated results were compared with experimental and calculated results obtained for these explosive substances earlier.

Determining combustion temperature of double-base solid propellants

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Keywords: solid propellant; burning test; temperature determination.

In the course of the testing aimed at determining the combustion temperature of double-base solid propellants, a series of five shooting experiments was conducted, consisting in the observation of the process of combustion with a high-speed video camera and determining the temperature on the basis of the obtained images in a specialist Thermias software. Based on the temperature field distribution histogram, the average, minimum and maximum values were determined for different moments in time.

Comparative study of Al/Ni intermetallic formed by planetary ball milling at different temperature

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Keywords: reactive material; intermetallic.

For fundamental understanding of morphological and thermal characteristics for Al/Ni intermetallic materials, we synthesized intermetallics composed of 31.5 wt. % of aluminum and the 68.5 wt. % of nickel by planetary ball milling at different temperature. The development of micro-structure phase between Al/Ni metals and compressive properties for compacts formed by the hydraulic press of prepared intermetallic powders under different pressures was investigated depending on the milling time and temperature. Moreover, the combustion behaviors of Al/Ni samples including the heat of combustion, the intensity of the reaction, and conformational/elemental change of compacts were compared with that of sample prepared at different temperature.

Experimental and theoretical investigation of the combustion heat of complex powders

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Keywords: comlex powders; heat of combustion; thermochemical calculations.

The main goal of the presented work was to check whether it is possible to use a thermochemical model to predict the heat of combustion of complex powders and to determine the calculation conditions that ensure obtaining the heat close to the calorimetric one. Calorimetric measurements of the heat of combustion of selected complex powders was carried out and their combustion characteristics were obtained from thermochemical calculations. The combustion heats determined experimentally and theoretically were compared. On the basis of the analysis of the obtained results, the approximate temperature of "freezing" of the composition of combustion products was established.

The Study of heterogenic high-energetic materials' combustion in laboratory rocket engine system

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Keywords: high-energy material; propellant; combustion attempt; pressure rate.

A series of attempts to initiate solid high-energetic materials inhibited by heat-shrinkable polyester film in the laboratory rocket engine system (LRE) were conducted in the research work. During the combustion tests of propellants, a sensor recording pressure changes vs. time was placed in the chamber of the LRE. The results from individual tests of propellant combustion were subjected to a comparative analysis.

Tensile test of HMX/HTPB macro-composites

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Keywords: PBX; adhesion; HMX; HTPB.

The adhesive and cohesive properties and the debonding of crystal/binder interfaces determine the mechanical behavior of a PBX under loading conditions. A new experimental approach has been done with the aim to measure the debonding of macroscopic binder/crystal composites in a tensile testing machine. Therefore Teflon sleeves were positioned on cm-sized HMX crystals, the binder, an HTPB/isocyanate mixture, was filled into the sleeves, screws were inserted headfirst into the still liquid binder, and the testing pieces were cured in an oven. The samples were measured after curing in a tensile testing machine equipped with a 10 kN load cell and the tests were monitored with a video system. The investigations revealed ultimate strengths, rupture energies, and yield points of the composites. However, various complications occurred during some tests such as tilted orientation of crystals, crystal cleavage or partial debonding. Details of the testing method, sample preparation, and evaluation are presented and discussed.

The exploration of the influence of cooling crystallization parameters on the characteristics of ammonium perchlorate particles: resolved by Taguchi orthogonal array design method

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Malek Ashtar University of
Technology, Tehran, Iran

Keywords: ammonium perchlorate; cooling crystallization; crystal size distribution; hardness; scanning electron microscopy; Taguchi's method; X-ray diffraction.

Please fill in (or paste)Crystallization is the most critical step in determining the mechanical strength and crystal size distribution of ammonium perchlorate. In this study, four crystallization parameters including cooling rate, cooling trend, mixing rate, and seeding ratio were selected and their effects on the bulk hardness and size distribution were studied by the implementation of Taguchi's method using a 1.3-litre agitated batch crystallizer. It is revealed that cooling rate was the most significant parameter in determining the bulk hardness of the resulted crystals where slower cooling rates resulted in greater bulk hardness and attrition resistance. The sub-180μ fraction of crystals was chosen to indicate the desirability of the size distribution of prepared products. This fraction and also average crystal size were mostly affected by seeding ratio. Taguchi's method was then employed to optimize the parameters toward maximizing the bulk hardness. Furthermore, scanning electron microscopy (SEM) and X-ray diffraction (XRD) were used for characterization of the harvested AP crystals. your abstract here. Use about 300 words.

Investigation of the effect of some polymers coating agent in the presence of CuCr2O4 and Fe2O3 nanoparticles on the thermal and safety properties of ammonium perchlorate particles

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Keywords: ammonium perchlorate; polymer coating agent; CuCr2O4 nanoparticle; thermal decomposition; safety parameters.

The purpose of this study was to improve the safety and thermal decomposition properties of ammonium perchlorate (AP) particles with microcapsulation by using some energetic fluorocarbon and nitro esters polymers containing viton A and nitrocellulose (NC) in the presence of CuCr2O4 and Fe2O3 nanoparticles as traditional burning rate modifier. Firstly, solution of polymers added to dispersed metal nano oxide in methyl ethyl ketone as wet media and subsequently, AP solution was added slowly to previous solution, and the microencapsulated particles was obtained by using a solvent evaporation method. Differential scanning calorimetry (DSC), thermogravimetry (TG) and scanning electron microscopy (SEM) techniques have been exploited to investigate the thermal properties, heat of decomposition and coating morphology of pure and treated samples. Evaluation of experimental results shown, the energy level for pure AP increased from 622 Jg-1 to1474 Jg-1 for treated samples. Also, SEM images shown, those samples with higher energy have a larger average particle size and suitable uniformity. the explosion propagation (EP) and sensitivity to shock (SS) for pure and treated ammonium perchlorate particles, respectively was calculated about -0.63 and -0.07 that confirm in contrast to increase in energy levels in treated sample, these safety factors included EP and SS remained less than zero that is desirable for AP as most common energetic material

DFT study on ammonium perchlorate bond activation by Pt clusters supported in the presence of carbon nanotubes and graphene

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Keywords: nanotube; ammonium perchlorate; clusters; transition metals.

Ammonium perchlorate (AP: NH4ClO4) is an oxidizer largely used in formulation of solid propellants because it is cheap and contains oxygen that generate stable reaction products in combustion reactions. Activation of the N–H bond of ammonium perchlorate is a vital channel for thermal decomposition mechanism. We investigated N–H bond breaking on Pt4 clusters supported by carbon nanotubes and graphene by using density functional theory method. In this study, comparison of (10-10), (8-8), (10-0) and (5-5) carbon nanotube models in zigzag and armchair forms was presented. As a result, opportune selection of size and chirality of carbon nanotubes supports can provide stable support for Pt clusters and to improve their catalytic activity.

Energetic materials derived from nitration of 3-amino-4-chloroximefurazan

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Keywords: furazan; energetic salt; nitramino.

Nitration of 3-amino-4-chloroximefurazan was performed with different nitration reagents, and different products were obtained. When N2O5 was used as the nitration reagent, a new fused compound potassium 6-nitro-pyrazolo-[3,4-c]furazanate-5-oxide was obtained. And when N2O5/N2O4 was used as the nitration reagent, nitration of 3-amino-4-chloroximefurazan followed by treated with KI/methanol gave rise to potassium 3-nitra-4-(dinitromethyl)furazan. A serial of energetic salts based on 3-nitra-4-(dinitromethyl)furazan anion were prepared and fully characterized.

Studies on hydroxychloride modification of phospholipids and its effect on reducing the viscosity of HMX-based PBX slurry

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Keywords: phospholipids; PBX; viscosity.

The viscosity has significant impact on the dispersion and forming process of polymer bonded explosive (PBX). Therefore it is important to reduce the viscosity of the slurry of PBX. Usually the surfactant is added into the slurry to reduce the viscosity. Phospholipid (1,2-dioleoyl-sn-glycero-3-phosphocholine, P1)is used as a sort of efficient surfactant .In this study, P1 was modified by hydroxychloride in order to enhance the viscosity reduction effect. The structure of hydroxychloride modified phospholipid (P2) was confirmed by IR spectroscopic analysis and NMR. By comparing the reduction of the surface tension of styrene before and after modification, it was proved that the two kinds of phospholipids could both reduce the surface tension of the styrene and the viscosity of the HMX-based slurry. And compound P2 had a superior viscosity reduction effect than P1. Moreover, the change of surface activity of the phospholipid after modification was studied by HLB value calculation.

Promising new insensitive cocrystal

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Keywords: EDNA; DAT; Cocrystal; sensitivity; EXPLO5 Code.

A novel energetic co-crystal based on 1,4-dinitro-1,4-diazabutane (EDNA) and 1,5-diaminotetrazole (DAT) in a 1:2 molar ratio was synthesized. The formation of the cocrystal was monitored by Scanning electron microscope (SEM), powder X-ray diffraction (PXRD) and Raman spectroscopy. Sensitivity to impact was measured and 50% probability of initiation was 9.73 J for the cocrystal and 15.4 J for the conformer EDNA. In addition, the detonation characteristics were predicted by EXPLO5 Code. The detonation velocity (D) and the detonation pressure (P) of the cocrystal are 8254.5 m s-1 and 26.7 GPa respectively. The obtained cocrystal possesses a promising future for expanding the reuse of EDNA in antitank ammunition after overcome the acidity problem in addition, the higher nitrogen content and acceptable sensitivity to external stimuli.

Simulations of the parameters influencing the underwater cutting systems availability and performance

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Keywords: high explosive; ANSYS; water pressure.

The motivation of this paper is to investigate the influence of different parameters on the efficiency of a linear shaped charge (LSC) ignited in an underwater environment. The efficiency of a LSC is determined by the maximal penetration depth into the tar-get. The capabilities of LSCs depend on various influencing factors directly linked to the geometry (apex angle, standoff distance, etc.). Therefore, considering this signifi-cant number of parameters that affect the penetration depth, the optimization of a LSC remains a really complex process. Some hydrocodes, such as Autodyn®, enable to simulate the jetting and penetration processes of the LSCs and to predict with a certain accuracy the maximal penetration depth into a target and the jet velocity.

Evaluation of concentration and type of fillers on the properties fluoropolymers compositions

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Keywords: energetic material; pyrotechnic; fluoropolymer; mechanical; fillers.

During operation, energetic materials are exposed to various types of influence (me-chanical, thermal, etc.). In order to ensure stability of operation in these conditions, it is necessary to know the basic dependence affecting on the characteristics of mate-rials. One of such factors is the interaction at the polymer-filler interface (the interac-tion surface area), structural grid of the filled polymer, etc. Therefore, a comprehen-sive assessment of the concentration, type and shape of the filler particles on the physico-mechanical characteristics and combustion characteristics of the pyrotech-nic system was made using the example of a fluoropolymer system.

Synthesis of 2,2-dinitroethene-1,1-diamine from 2-methylpyrimidine-4,6-diol and treatment of dinitromethane formed

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Keywords: 2,2-dinitroethene-1,1-diamine; dinitromethane.

2,2-Dinitroethene-1,1-diamine was prepared from 2-methylpyrimidine-4,6-diol. Dinitromethane that forms was disposed by heating in dilute sulphuric acid or by using of reducing agent. Analytical methods for identification of dinitromethane content are described.

Dust Explosion of two delaying compositions in 20 l Chamber

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Keywords: energetic material; dust explosion; delay composition; 20 l chamber.

There is a lot of situation during manufacturing of solid energetic materials where flammable dusts containing explosives and/or materials categorised as explosives are produced. This brings a problem with potential development of dispersion of dust containing those materials. Dust dispersion of two delaying compositions were tested in 20 l chamber. Maximum explosion pressure and maximum rate of pressure rise were measured. It was proved by tests that dust dispersion of multi-component composition behaves in a different way comparing to bulk of that composition. Safety and health protection of workers potentially at risk from explosive atmospheres, and flammable dust dispersions are categorized as explosible atmosphere, is regulated by a Directive 1999/92/EC of the European Parliament and of the Council of 16 December 1999 on minimum requirements for improving the safety and health protection of workers potentially at risk from explosive atmospheres. Unfortunately, this Directive shall not apply to "the manufacture, handling, use, storage and transport of explosives or chemically unstable substances". Explosives authorities, Standards and laws do not treat those explosible atmospheres. Then who should and who should test them?

Influence of different components on the sensitivity to impact of TATP and HMTD

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Keywords: TATP; HMTD; reduced impact sensitivity.

TATP and HMTD belong to the class of organic peroxide explosives and are highly sensitive to mechanical impulses. They can be synthesized from easily available precursors and can be therefore used as improvised explosives. Thus organic explosives are frequently the subject of disposal procedures performed by EOD teams worldwide. The risks during the disposal procedure are due to the high brisance and high sensitivity of the explosives. Using a method to decrease the friction and impact sensitivity of TATP and HMTD will decrease the risk of the disposal procedure. Friction and impact occur during practically all type of manipulation: transfer of the explosive, stirring, transportation. . . Methods to decrease the sensitivity to friction have been investigated by R. Matyas. In our work, we investigate methods to decrease the sensitivity to impact of TATP and HMTD. Different components have been tested. The adding of water mixed with a detergent has shown no positive effect; in fact in a test the impact sensitivity of the mixture was higher than of the pure TATP. We speculated that this is due to the formation of air bubbles in the mixture. The adding of methanol, ethanol, toluene, acetone, diesel and WD40 has been tested. Ethanol successfully flegmatizes the TATP but also dissolves the explosive and by consequence it cannot be easily manipulated. Methanol, acetone and WD40 decrease the sensitivity to impact of TATP and HMTD but the impact sensitivity of the mixture or of the solution is still lower than 2 J which is the limit at which a substance can be considered as safe for transportation, considering the impact sensitivity criteria. Diesel and toluene does not decrease the impact sensitivity of the TATP or HMTD and in some case a higher sensitivity than the one of the pure TATP or HMTD is obtained. This is an important result as diesel is often used to flegmatize TATP or HMTD by EOD teams.

Dibenzoyl peroxide - the study of sensitivity to simple stimuli and its desensitisation

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Keywords: dibenzoyl peroxide; impact; friction; electric spark sensitivity; desensitisation.

Dibenzoyl peroxide is one of the most widely used and manufactured peroxy com-pounds. It is commonly employed in a large number of organic syntheses, polymeri-sation procedures, as well as in the curing of resins, polyesters and silicone rubbers. It has also found application in the pharmaceutical and food industries. Inde-pendently of its common usage, it is a highly flammable and oxidising substance, posing a severe potential fire and explosion threat. The widespread demand for this substance requires large volume manufacturing, storage, handling and transport. As such, ensuring the safety of working and handling this compound is of critical im-portance. This report presents the results of dibenzoyl peroxide sensitivity tests, con-ducted for simple stimuli (impact, friction, electrostatic discharge) and our attempts to desensitize the compound via the use of ethylene glycol dibenzoate, glycerol tribenzoate and dicyclohexyl phthalate.

Modeling of thermochemical characteristics and crystal structure of mesoionic compounds

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Keywords: high-energy compound; atom-atom potential method; sintone; oxatriazolium-5-aminide; tetrazolium-5-olate; molecular electrostatic potential; crystal structure; sublimation enthalpy.

The thermochemical characteristics of a set of 1,2,3,4-oxatriazolium-5-aminides and isomeric 1,2,3,4-tetrazolium-5-olates were investigated experimentally and some of them were modeled. Using Atom-Atom Potentials Method (AAPM), the crystal package and the enthalpy of sublimation of one of the compounds considered were predicted and results were obtained in good agreement with the experimental data.

Modeling of the crystal structure of multifurazan compounds by the example of bifurazano[3,4-b:3',4'-f]furoxano[3'',4''-d]oxacycloheptatriene (BFFO)

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Keywords: high-energy compound; atom-atom potential method; HF/6-31G(d, p) calculation; molecular electrostatic potential; crystal structure; sublimation enthalpy; molecular crystal density.

Modeling of the crystal structure of bifurazano[3,4-b:3',4'-f]furoxano[3'',4''-d] oxacycloheptatriene (BFFO) has been carry out using the original technique of optimized point charges approximation of the molecular electrostatic potential (MEP) obtained from ab initio calculations. The best models were used to calculate the crystal packing of the molecules within the framework of AAP method with the refined parameters of Lennard-Jones potential ("6-12"). The optimal packing and density of molecular crystal of BFFO) have been determined.

Crystallization of nitramine energetics by drowning-out

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Keywords: crystallization; drowning-out; RDX.

Nanonization of RDX (cyclotrimethylene trinitramine) by drowning-out has been studied because of the insensitiveness effect of RDX particles arising from the size reduction aiming toward invulnerable munitions. In the present work, effects of antisolvents, solvent/antisolvent pairs, mass ratios between them on the average size of RDX particles were enumerated. Sub-micron sized particles was precipitated out by crashing of RDX solution into antisolvent. Such important variable on reducing particle sizes was the mass ratios of solvent and anti-solvents which mainly forced the RDX solution out the high supersaturation. Experimental results showed that sub-micron particles below 1 um was attained from right combination of solvent and anti-solvent.

Energetic copper(II) bromate complexes as replacement of lead and perchlorate containing primary explosives

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Keywords: energetic copper(II) bromate complex; laser ignition; lead-free primary explosive; N-heterocycles; structure elucidation.

The strong oxidizing power of the bromate anion in combination with nitrogen-rich ligands was used to prepare six new energetic copper(II) coordination complexes. The compounds were investigated as a replacement for lead and perchlorate containing primary explosives. For the characterization, all complexes were analyzed (XRD, EA, IR and DTA) and tested toward their sensitivities (IS, FS and ESD). Promising complexes were examined on their suitability as possible primary explosives in laser ignition experiments hot plate and hot needle tests. Furthermore, solid state UV-Vis measurements were accomplished to get a better understanding of criteria important for the laser initiation.

Design of polynitro substituted azapropellane derivatives and their synthetic exploration

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Keywords: azapropellane; nitration.

Design and synthesis of polynitro strained-ring/cage based molecules are highly demanding in the field of energetic materials. In our work, eleven polynitro substituted azapropellane derivatives are designed and their energetic properties are computationally analysed. Densities are evaluated from Material Studio (v.08) and heats of formation of designed molecules are calculated from semi-empirical method using MOPAC16. The detonation properties are predicted using Explo5 version 6.03. Theoretically predicted energetic properties of molecules showed high densities (1.81 to 2.10 g/cc) and excellent detonation properties (8054 to 9590 m/s; 28 to 42 GPa). Synthetic studies of few designed molecules are discussed.

Enthalpies of formation of derivatives phenylazasidnones

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Keywords: calorimetry; energy of combustion; enthalpy; azasidnone; nitrophenyl group.

The method of calorimetry of burning in oxygen atmosphere has been used for measuring of combustion energy of some new nitrogen-containing compounds - derivatives phenylazasidnones. On the basis of the received values enthalpies of combustion and formation in a standard condition of the investigated compounds are defined. The got data on enthalpies formation of phenylazasidnones it is possible to use for an estimation of power characteristics of new compounds.

Thermal decomposition kinetics of 3-nirto-5-R-1,2,4-triazoles in solutions

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Keywords: 3-nitro-5-R-1,2,4-triazoles; thermal decomposition; autoprotolysis; solvent dielectric permittivity.

Thermal decomposition kinetics of some 3-nitro-5-substituted 1,2,4-triazoles has been studied in solutions of dinitrobenzene, trinitrobenzene, dibutyl sebacate, and dibutyl phthalate by the manometric method. The rate constant of decomposition decreases with solution dilution and is effected of the solvent's dielectric permittivity. Kinetic parameters of the compounds are similar and significantly different from those for homolysis of bonds C-NO2, C-N and N-N in the azole ring. With this in mind, autoprotolytic thermal decomposition mechanism is postulated, which is confirmed by kinetic analysis.

Detonator testing using photonic Doppler velocimetry

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Keywords: detonator; initiation; free surface velocity; photonic Doppler velocimetry.

The paper describes a method for characterization of detonator output using photonic Doppler velocimetry (PDV). Initiation of explosive charges by the shock-to-detonation transition takes place in a majority of practical applications. Successful initiation of an acceptor explosive depends on the incoming shock pressure and its duration, i.e. the energy fluence. Industrial electric detonators with copper and aluminium casings were tested using custom made 3D-printed holders. The PDV instrumentation allowed us to obtain free surface velocity profiles at specific areas of the detonator's casing. The proposed measurement setup may also be useful for characterization of small samples of newly developed high explosives.

Dispersed dusts studies: pyrotechnic compositions for igniter

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Keywords: pyrotechnic; igniter; dispersed dust.

Chemical igniters are used in the study of dispersed dusts. Energy released during use is defined by EN 14034 at 2 x 5 kJ. The standard does not define the exact composition of the pyrotechnic mixture, so it is possible to use non-standard igniter fillings. The condition of using the lighter is to release energy according to the standard. This article focuses on selected pyrotechnic compositions with the ability to ignite the dispersed dusts that were designed on Department of Safety Engineering. The article discusses their composition, the ignition timing and how the igniter is arranged. These values are important for setting up a device for studying the explosive properties of dispersed dusts.

Sensing of some interesting NACs through fluorescence quenching studies

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Keywords: sensing; fluorescence quenching.

The development of reliable detection of explosives is one of the pressing concerns in anti-terrorism efforts and environmental pollution controls. Different sensors have been developed for detection and trace detection of explosive materials and High energy Materials (HEMS). However these are found to have limitation in terms of cost and easy adaptability. In recent studies fluorescence-based sensing technology has emerged as one of the most promising approaches for trace explosives detection due to the advantages such as short response time, excellent sensitivity, and instrumental simplicity. Herein, we report the synthesis of camphor sulfonic acid doped polyaniline (CSA-PANI) synthesised through chemical route and its characterization employing various experimental tools. We report the efficiency of our CSA-PANI as fast, sensitive, selective, reliable and cost effective material for detection of nitro-aromatic explosives (NACs) like picric acid and para nitro toluene. The successfully demonstration through fluorescence quenching of conjugated polymers of NACs is envisaged with N-methyl pyrrolidone as solvent. Quenching efficiency has been estimated by Stern−Volmer equation. The mechanism for the ultrasensitivity of CSA-PANI to detect PA is attributed to the "molecular-wire effect", through photoinduced electron transfer (PET) process is evidenced from spectroscopic and redox studies.

Organic solvent-free water slurry coating : Effects of pre-heat treated polyacrylate emulsion and additional additives

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Keywords: press PBX; organic solvent-free water slurry coating.

We firstly developed the organic solvent-free water slurry coating(OSF-WSC) method for press PBXs by direct use of polyacrylate emulsion and concluded from previous results that their sensitivities weere similar irrespeictive of preparation methods between existing WSC and newly developed OSF-WSC method. In this work, we investigated the effects of pre-heat treated polyacrylate emulsion at 80'C and additional additives such as talc and graphite on their morphology, compressive properties, and sensitivities of PBXs prepared at same composition using OSF-WSC.

Characterization of polyester-based polyurethane elastomers plasticized with energetic ionic liquids

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Keywords: energetic ionic liquid; EIL plasticizer; Desmophen binder; polyester binder; DMA; thermogravimetry.

Energetic ionic liquids (EILs) were used as plasticizers in polyester-polyol based polyurethane elastomer samples. The polyol was Desmophen® D2200 cured with Desmodur® N3400. The elastomer samples were characterized in terms of dynamic mechanical properties, tensile strength and thermogravimetry. The EIL samples are based on 4-Amino-1-alkyl-1,2,4-triazolium nitrate and are mixtures with different alkyl length, named aN1 and bN2. The first is a mixture containing longer alkyl substituents (4, 6 and 8 carbons), whereas the second one has shorter alkyl substituents (1 and 4 carbons). The addition of ionic liquids to the elastomer did not affect the main glass-rubber transition temperature (T_g) of the binder. However, the dynamic mechanical properties are changed especially after T_g. Tensile testing showed that at ambient temperatures the addition of ionic liquids increased substantially the strain capability of polyester-based polyurethane binder. In the case of the addition of molecules with shorter aliphatic substituents, also higher maximum tensile stress is achieved. EILs as plasticizer impart a very soft rubbery behaviour to the binder, reflected also by the decrease in Young moduli. Thermogravimetry analysis showed a relatively high thermal stability of the EILs compared to other common energetic plasticizers in the elastomer bulk.

Standard enthalpy of formation of some nitropyrazolyltetrazoles

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Keywords: enthalpy of formation; nitropyrazolyltetrazoles.

The experimental values of the heats of combustion ($\Delta H^{\circ}c$) and standard enthalpies of formation ($\Delta H^{\circ}f$) for some isomers of nitropyrazolyltetrazoles have been determined. The quantitative contribution of some energetic groups into the total $\Delta H^{\circ}f$ value of the compounds have been determined. These data may be used for a correct evaluation of the $\Delta H^{\circ}f$ values of known energetic compounds as well as of hypothetic ones.

Thermochemical and energetic properties of a couple of azidoderivatives of terfuranans

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Keywords: energetic compound; enthalphy of formation; azide; furazan; ballistic effectiveness.

The experimental values of the heats of combustion (△H°c) and standard enthalpies of formation (△H°f) for two compounds (3,4-bis(4-azidofurazan-3-yl)furoxan — DAzFF, and 4-azido-4′′-nitro-3,3′:4′,3′-terfurazan — AzNTF) have been obtained: △H°c=-3666.2±4.5 kJ/mol, △H°f =1305.1±4.5 kJ/mol for DAzFF and △H°c=-3319.1±4.6 kJ/mol; △H°f =958.0±4.6 kJ/mol for AzNTF. It has been shown that for creation metal-free solid composite propellants basing on AzNTF or DAzFF one should use active binders and introduce a small amount of an oxidizer with a high oxygen content, e.g. ammonium perchlorate. Such compositions have equal or even higher energetic characteristics in comparison with similar ones basing on HMX.

The investigation on the properties of TNBI and its salts

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Keywords: energetic material; synthesis; explosive properties; TNBI.

The main purpose of this study was to synthesis new ionic derivatives of 4,4',5,5'-tetranitro-1H,1H'-2,2'-biimidazole (TNBI) which can be used as modern secondary explosives. Firstly, an attempt was made to fully characterize TNBI dihydrate. The compound was examined with spectroscopic methods, elemental analysis, thermal analysis and small scale safety testing (impact and friction sensitivity). The results of experimental investigation of explosive properties of TNBI•2H2O were also presented. Non-isothermal kinetics analysis, calorimetric measurements, detonability tests, detonation velocity measurements and cylinder tests were performed. Results of the cylinder tests were used to determine the acceleration ability of TNBI•2H2O detonation products. The known salts of TNBI with guanidine, aminoguanidine, diaminoguanidine, triaminoguanidine and ammonia were obtained to confirm their interesting properties. The group of the new compounds includes salts with semicarbazide, carbohydrazide, acetamidine, adenine, cytosine, 3-amino-1,2,4-triazole, 4-amino-1,2,4-triazole, 3,5-diamino-1,2,4-triazole and 5-aminotetrazole. The structure of the molecules was proposed on the basis of the results obtained by methods of nuclear magnetic resonance and elemental analysis. Thermal properties were examined by differential thermal analysis and thermogravimetry. In order to determine the safety of the production and use of the new compound sensitivity to impact and friction tests were performed. Detonation parameters were calculated with CHEETAH code for density determined for pressed sample of TNBI dihydrate. The explosive properties were determined for the TNBI salt with semicarbazide. This compound was selected for the further investigation because of its insensitivity, high theoretical detonation parameters and inexpensive synthesis. The study showed that the salt could be used as a secondary explosive material but it has lower detonation parameters and acceleration ability than 2,4,6-trinitrotoluene.

Investigation of the tautomerism of imidazo[4,5-e] benzo[1,2-c, 3,4-c]difuroxan derivatives by computational and experimental methods

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Keywords: furoxan; tautomerism; NMR; LC-MS; DFT.

The tautomerism of the energetic tetracyclic system derivatives (imidazo [4,5-e] benzo [1,2-c, 3,4-c '] difuroxan) in DMSO-d6 at the room temperature and in the water-acetonitrile-formic acid system have been investigated using NMR (1N, 13S) and liquid chromatography/mass spectrometry. The structure and thermodynamic characteristics (formation enthalpy (ΔHf0) and Gibbs energy (ΔG)) of these compounds have been calculated by quantum-chemical methods (DFT B3LYP / 6-311 ++ G **) and the relative thermodynamic stability of their tautomeric forms has been estimated. The effect of substituents and their position on the equilibrium of tautomers in the solution has been evaluated.

Detonation velocity of selected mining explosives using MicroTrapTM VOD/Data Recorder

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Keywords: hydrogen peroxide; heavy ANFO; emulsion explosives; detonation velocity; MicroTrapTMVOD/Data Recorder.

Explosive velocity also known as velocity of detonation (VOD) is one of the most important and basic parameters describing the properties of explosives. VOD is the velocity at which the shock wave front travels through a detonated explosive. The amount of heat generated in the chemical reaction zone of the detonation wave indicates the possibility of using an explosive to perform specific blasting operations. Ionisation sensors and electro-contact ones can be used for continuous measurement of detonation velocity. These are used in the MicroTrapTM VOD/Data Recorder which was used in presented research. The aim of the experiments was to investigate the development of detonation processes in new explosives based on concentrated hydrogen peroxide (HP), emulsion explosives and heavy ANFO.

Study of thermal decomposition of coated oxidizer based composite solid rocket propellants

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Keywords: oxidizers; coating; ammonium perchlorate; porous ammonium perchlorate; nitrocellulose.

The objective of this work is to study the effect of coating of different oxidizers : normal, porous, normal coated with NC and porous ammonium perchlorate coated with NC on thermal decomposition and thermokinetic parameters of the combustion using the differential scanning calorimetry method. The first part of this study is to present the experimental procedure concerning the coating of oxidizing charges and their characterizations. The second part will be dedicated to the kinetic study of oxidizing charges. The purpose of the latter is to evaluate and determine the different kinetic parameters (the activation energy, the pre-exponential factor and the kinetic model). in order to determine thermal parameters and kinetic data (activation energy, frequency).

Synthesis of hyperbranched polyglycidylnitrates

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Keywords: hyperbranched polyglycidol; nitration; IR spectroscopy; NMR; chain structure.

Synthesis, study of properties and practical application of hyperbranched polymers is one of the directions of development of modern polymeric material science. Hyperbranched polymers can contain a large number of different functional groups, which makes them interesting objects for polymer-analogous transformations. Promising representatives of polymers of this class are hyperbranched polyesters containing numerous hydroxyl groups. Such dendrimers can be prepared, for example, by polymerization of glycidol. Nitration of such hyperbranched polyesters is one of the directions in the synthesis of hyperbranched energy polymers. The methods for obtaining such polymeric structures and studying their properties have both fundamental and applied significance, since they can significantly affect the characteristics of energy polymer systems. As a result of the study, branched polyglycidyl nitrates (PGN) of various structures were obtained, their structure was determined and it was proved that nitration does not lead to the destruction of polymer chains. The work was supported by the Program of Basic Research of the Presidium of the Russian Academy of Sciences No. 56.

Influence of the sizes of gunpowder units reused in industrial water-gel explosives on detonation characteristics

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Keywords: slurry explosive; water gel explosive; detonation; industrial explosive; single base propellant.

Reuse of expired single base propellants from munition as component of industrial explosives is one of energy saving technologies. In this paper the data on study influence of gunpowder units of various sizes in a mixture with a water-gel composition on detonation by the electromagnetic method are presented. The increase of the size of gunpowder units promotes increasing of detonation velocity despite the loss of the mass fraction of the gunpowder in the charge. Typical profiles of detonation pressure depending on various sizes of gunpowder units are presented. The features of detonation depending on the size of the gunpowder units are described.

Use of microcalorimetry to assess the stability of single base propellants

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Keywords: single base propellant; stability; microcalorimetry; heath flow; lifespan.

This study deals with the assessment of the stability of six single base propellants samples having various ages. Various methods of analysis and characterization have been carried out, like the high performance liquid chromatography (HPLC) for the qualitative identification and the quantitative evaluation of stabilizers contained in propellants, the FTIR spectroscopy, which allows via the detection of the vibrations characteristic of the chemical bonds, to carry out characterization of chemical functions, and the determination of density of the different propellants samples. The essential part of this study consists of an attempt to develop methodology allowing the study of the stability of single base propellants by using microcalorimetry technique in isothermal mode. Thermal Activity Monitor (TAM III) device is used throughout this study for the achievement of experimental work. An important part of work consists with the assessment of the lifespan of propellants by using various well known empirical models for these energetic materials.

High-molecular block copolymers of nitrateomethyl and azidomethyl substituted oxetanes

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Keywords: 3,3-bis(azidomethyl)oxetane; 3- nitratomethyl -3-methyloxetane; 3-azodomethyl-3-methyloxetane; block copolymers; cationic ring opening polymerisation (CROP).

The article presents the results of research of synthesis block copolymers nitratomethyl and azidomethyl-substituted oxetanes. 3- nitratomethyl -3-methyloxetane and 3,3-bis(azidomethyl)oxetane, 3-azodomethyl-3-methyloxetane and 3,3-bis(azidomethyl)oxetane copolymers have been synthesized with different amount of monomer units. As a catalyst trialkylaluminum-water system with 1:0,8 ratio was used. Copolymers were investigated by FTIR, differential scanning calorimetry, viscometry and elemental analysis.

MD simulation of HMX rupture under tensile stress

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Keywords: MD simulation; HMX; mechanical properties; plasticity.

Determination of the boundary of the elastic regime for beta-HMX with its plasticity threshold is hardly accessible by experimental methods, and mostly estimated from crystal indentation or impact tests on composites or pressed powders. It is commonly accepted to be highly anisotropic and dependent on deformation speed. To establish a traction-separation law for internal grain damage in prospective finite-element modelling, molecular dynamics simulations (MD) of tensile tests are conducted on an atomistic scale. Goals are: 1) Compare stiffness in the elastic regime at small deformations with experimental values. 2) Determine the plasticity threshold for intermediate deformation. 3) Simulate the full stress-strain curve until complete rupture to determine the extent of the amorphous regions formed in the transition to crack and on the exposed crack surface. Results are presented for axial tensile tests in crystallographic direction b of beta-HMX. The MD model corresponds to a free standing crystalline (nano-) rod with principal axis b that is gradually elongated, while stress, work of deformation and (decreasing) degree of crystallinity are measured as a function of strain. In concordance with experimental findings, the linear elastic deformation of the crystallographic b axis of beta-HMX shows a slope in modulus of roughly 15 GPa, until a stress maximum of 0.3 GPa is reached at a strain of 2%. Further strain results in a stress plateau at 300 MPa, where molecular rearrangement occurs within a plane perpendicular to the b-axis, at the outer region of a rod-shaped specimen, which corresponds to plastic deformation. At a strain of 0.28, the peel-like rupture is completed.

Specific features of thermal decomposition of organic azides

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Keywords: heterocyclic azides; thermal decomposition; carbon-nitride materials; kinetics; mechanism; cyanuric triazide; impact sensitivity.

The kinetics, mechanism, and products of thermal decomposition of nitrogen bearing heterocyclic azides in a melt and in a solution have been studied. The results obtained, together with literature data, indicate that the mechanism of decomposition of a heterocyclic azide depends significantly on its structure. If the azide molecule does not contain hydrogen, then the intermediate nitrene cannot enter into its characteristic hydrogen abstraction reaction. As a result, the decomposition mechanism and kinetic parameters of the reaction change; in particular, the values of the pre-exponential factor increase. Intermediate nitrenes can be relatively long-lived. The change in the reaction mechanism results in a change in the composition of the condensed products: during the decomposition, both linear oligomers and flat polyconjugate carbon-nitride networks can be formed. The results obtained were used to explain the cause of a high impact sensitivity of cyanuric triazide. It turned out that the high sensitivity is kinetic but not thermodynamic in its nature.

Synthetic studies on HNIW

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Keywords: HNIW; composite fuel.

HNIW (2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaiso wurtzitane) is a high-energy nitramine based molecule used in explosive formulation of rocket motor fuel and warheads. Due to its positive heat of formation value, it is used in the production of high energy and smokeless composite fuel. In the synthesis of this molecule, various laboratory studies have been performed to improve the conversion rate (yield). In this study, HNIW was initially synthesized in lab scale to optimize its production parameters, which were then applied for a medium scale production.

Fluorescence quenching studies of picric acid, employing PTSA doped polyaniline

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Keywords: doped polyaniline; picric acid; fluorescence quenching; sensing.

Polyaniline (PANI) was synthesized by chemical oxidation polymerization method in the presence of ammonium persulfate as oxidant and para toluene sulphonic acid (PTSA) as dopant. In this study, fluorescence characteristics of polyaniline doped with PTSA in Dimethyl sulfoxide (DMSO) as solvent is under taken. The synthesized PTSA-PANI is characterized for its structure, morphology and thermal behaviour employing spectroscopic, thermal, SEM and X-RAY instrumental techniques. The detection of quencher (Picric acid) is studied through the observed intense quenching of fluorescence signals in the emission spectra of the PTSA-PANI solution. The limit of detection of quencher in the polymer solution is found to be 100 ppm for 100 ppm of PTSA-PANI solution.

The blocking effects of inert impurities on thermo-mechanical response of α-RDX under shock stimuli: a CGMD study

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Keywords: energetic crystal; impurity; molecular dynamics; shock; thermo-mechanical response.

In energetic crystals, chemically-inert impurities such as inert-metal or dust may exist inside the crystal due to the fabrication process. Nevertheless, the effects of these inert-impurities on the performance of energetic crystals were rarely paid attention to. In our study, a coarse-grained molecular simulation method was applied on the impurity-contained alpha-RDX under shock stimuli, both the nano-solid sphere model and nano-solid gap model were considered, and the evaluation of local stress field, temperature field, meso-scale damages as well as axial stress/temperature distributions along shock direction were obtained and compared to that of the pure RDX. The results show that the stress distributions were heavily effected by the impurity, peaks can be found in the region of the impurity, and the localization of stress can also be found; the effects of the nano-sphere on the temperature distributions were not so obvious, meanwhile, the inert gap can block the propagation of heat,then inducing the localization of high temperature. The above prove the blocking effects of inert impurities on the thermo-mechanical response for RDX, which is related to the safety and detonation properties of the energetic crystals.

Energetic characteristics of CuTNO

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Keywords: explosive materials; complexs; TNBI derivatives.

The aim of this work was to investigate explosive characteristics of an energetic complex CuTNO which contain copper as coordination centre and 4,4',5,5'-tetranitro-2,2'-biimidazole (TNBI) as a ligand. Properties of the title compound were examined with nuclear magnetic resonance methods, elemental analysis and atomic absorption spectroscopy. Characteristics as the ability to detonation, velocity, activation energy, thermal stability or thermodynamic parameters were determined. Sensitivity to impact and friction were tested also.

Energetic 3-nitramino-triazole derivatives

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Keywords: explosive; triazole; nitrogen-rich; sensitivity; crystal structure.

The synthesis of several nitrogen-rich 3-nitramino-1,2,4-triazole derivatives is described. Triazole based compounds offer several benefits over conventional energetic materials, such as high heat of formation, high density and thermal stability. The obtained compounds were characterized via multinuclear NMR and IR spectroscopy, mass spectrometry, elemental analysis, DSC measurements and single crystal X-ray diffraction. The sensitivities toward external stimuli (impact, friction and electrostatic discharge) were determined according to Bundesamt für Materialforschung (BAM) standard methods. The energetic properties have been calculated with the EXPLO5 computer code using recalculated X-ray densities. Solid-state heat of formation were calculated using the CBS-4M atomization method.

New N-heteryl derivatives of tetrazolo[1,5-b][1,2,4,5]tetrazin-6-amine

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Keywords: tetrazolo[1,5-b][1,2,4,5]tetrazin-6-amine; [1,2,4]triazolo[4,3-b][1,2,4,5]tetrazines; 1,2,4,5-tetrazines; nucleophilic substitution; azido-tetrazole tautomerism.

New energetic derivatives of tetrazolo[1,5-b][1,2,4,5]tetrazin-6-amine have been synthesized by nucleophilic substitution reactions. All compounds were identified by FTIR, 1H, 13C NMR spectroscopy and LC-MS analysis. The thermal stability of new materials was estimated by differential scanning calorimetry and their energetic characteristics were calculated.

Physico-chemical properties and combustion behavior of new oxygen-rich pyrazolyltetrazoles

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Keywords: decomposition kinetics; N-[3-nitro-1-(trinitromethyl)-1H-pyrazol-4-yl]-1H-tetrazole; N- [1-(fluorodinitromethyl)-3-nitro-1H-pyrazol-4-yl]-1H-tetrazole; combustion; vapor pressure.

Physico-chemical characterization of new oxygen-rich N-[3-nitro-1-(trinitromethyl)-1H-pyrazol-4-yl]-1H-tetrazole (1) and N- [1-(fluorodinitromethyl)-3-nitro-1H-pyrazol-4-yl]-1H-tetrazole (2) has been conducted, including studies on the thermal decomposition, burning behavior, and flame structure. It was found that the trinitromethyl group and the tetrazole substituent have a close thermal stability and decompose simultaneously under the nonisothermal conditions (DSC experiments). The fluorodinitromethyl fragment is more stable than the trinitromethyl group, the decomposition of this substituent and the tetrazole ring proceeds at different temperature intervals under the conditions of DSC tests. It turned out that pyrazolyltetrazoles have high burning rates. The structure of the combustion wave of compound 2 was determined with the help of thin thermocouples. Combustion of the investigated substances obeys the combustion model with the leading reaction in the condensed phase due to their high decomposition rates. In the case of compound 1, the leading reaction is the decomposition of the trinitromethyl group and the tetrazole moiety, and in the case of compound 2, the combustion rate is determined by the decomposition kinetics of the more stable but more energy-rich fluorodinitromethyl group, since rapid release of heat upon the tetrazole moiety decomposition is insufficient to maintain combustion.

Primary thermolysis reactions of 3,3'-diamino-4,4'-azofurazan (DAAzF) thermal decomposition: a CCSD(T)-F12 study

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Keywords: furazan derivative; high-energy compound; thermal decomposition; highly accurate quantum chemical calculation; computational kinetics.

Primary reactions of thermal decomposition of diaminoazofurazan (DAAzF), a promising insensitive explosive, were studied theoretically at a high reliable level of theory (CCSD(T)-F12). The most favorable thermal decomposition channel is a concerted molecular elimination of cyanamide from a trans-isomer of DAAzF with the Arrhenius parameters of the rate constant log A = 14.7, Ea= 52.4 kcal/mol. The radical decomposition channels of DAAzF are highly endothermic (>70 kcal/mol) and are not important for thermolysis mechanism. All reactions of a cis-isomer of DAAzF turned out to be kinetically unimportant as well.

Features of thermal decomposition of N-substituted tetrazoles

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Keywords: decomposition kinetics; pyrazolyltetrazoles; combustion; vapor pressure.

In recent years, the concept of creating molecules that are a combination of several heterocycles is widely used. This approach allows to obtain compounds with new properties that expand the field of their application. Many tetrazole derivatives have high combustion rates. The introduction of the tetrazole fragment into the composition of the nitropyrazoles led to the synthesis of new fast-burning compounds. Investigation of the thermal stability of new pyrazolyltetrazoles showed that the decomposition of molecules begins with the decomposition of the tetrazole fragment, and the stability of the substances decreases with increasing electronegativity of the pyrazole substituent. The flame structure of new pyrazolyltetrazoles was studied with the help of thin microthermocouples. It turned out that the decomposition reaction in the condensed phase controls the burning rate of these compounds.

Influence of catalysts on the burning rate of nitrocellulose

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Keywords: nitrocellulose; burning rate; catalysis; carbon materials; carbon nanotubes.

Nitrocellulose is an essential part of single- and double-based propellants. But some questions remains in the catalysis of nitrocellulose. It is known that for the catalysis of double-based propallant carbon frame is needed. It can be formed from nitrocellulose in the low-calorie propallants or when we add carbon to the composition of propellant. In this work influence of carbon materials and some catalysts on the nitrocellulose with various content of nitrogen is investigated. It is shown that the higher the content of nitrogen (from 12 to 13,5%), the harder to catalyze the nitrocellulose. Some efficient catalysts show no result on the burning rate of the nitrocellulose.

Synthesis of ferrocenedicarboxylic acid as a primary component for burning rate catalysts

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Keywords: ferrocenedicarboxylic acid; burning rate; catalysis.

The preparation of ferrocenedicarboxylic acid and optimization of synthesis based on previously known is described. Some source components need prior preapration. From the resulting acid obtained its salts, which are used as burning rate catalysts for nitrocellulose and propallants on its basis.

Influence of carbon nanotubes on the catalysis of propellant

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Keywords: burning rate; propellant; ammonium perchlorate; carbon nanotubes; catalysis.

The regulation of the burning rate and its dependence on pressure is one of the primary tasks when composing the propellant. Propellants on the basis of ammonium perchlorate (AP) and polymer binder are difficult to catalize. One of the methods is varying the particle size of AP. Another - use of various additives. It is known that carbon materials are essential in the catalysis of double-based propellants but its effect on the catalysis of AP-based propellant studied is not good enough. That's why the effect of various carbon materials, such as carbon black and multi-walled carbon nanotubes on the burning rate of the propellant was studied. Carbon materials were added into the propellant as an independent additive and together with catalysts. In this work, catalysts such as copper oxide (CuO) and iron (III) oxide (Fe2O3) and carbon materials in amount of 1-3% were used.

Physicochemical properties of 2-nitro-2-azidomethylene-1,3-diazidopropane

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Keywords: nitro-2-azidomethylene-1,3-diazidopropane; glass temperature; temperature and enthalpy of thermal decomposition; constant of thermal decomposition; burning rate.

Physicochemical properties of 2-nitro-2-azidomethylene-1,3-diazidopropane have been studied. The glass temperature, temperature and enthalpy of thermal decomposition, and thermal stability of 2-nitro-2-azidomethylene-1,3-diazidopropane have been determined using differential scanning calorimetry. The glass temperature is -85° C. The temperature and enthalpy of decomposition are 231°S and 1665 J/g. An equation has been derived for the constant of 2-nitro-2-azidomethylene-1,3-diazidopropane thermal decomposition. Factor 0k = 2.03×10 8 s -1 and activation energy of thermal decomposition E =101.02 kJ/mol. The-2-nitro-2- azidomethylene-1,3- diazidopropane are completely thermodynamically compatible with polyurethane and divinylnitrile rubbers ,cellulose nitrate(12 % N) and polyvinilnitrate. Double-based propellant was produced and burning rate is determined with this plasticizer as a partial replace of nitrooglycerine. The possibilities of propellant catalysis were investigated.

Low-sensitivity PETN crystallized in a presence of stearic acid

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Keywords: PETN; RDX; LOVA; stearic acid.

Crude PETN was co-precipitated with 1% of stearic acid from acetone solutions. Final product contained approx. 0.2-0.3 % of stearic acid (SA). Material was found to be surprisingly significantly less friction sensitive than PETN precipitated without stearic acid (72-84 N with SA, 42-48 N without SA). Impact sensitivity was also reduced from 5-7.5 J to 10 J level. Stability and melting point were not affected by small quantity of stearic acid, nevertheless crystals were more spherical with low amount of crystal defects. Because of promising safety characteristics of this product similar to RDX, 400 kg batch of this PETN was prepared and tested for manufacture of blasting cord and polyethylene-coated product for blasting caps and cord. This crystallization technique seems to be effective for safer handling with dry PETN in manufacture of initiators and plastic explosives. Safer products for military applications can be also produced. Explosia a.s. is now testing and evaluating big scale production of these products with lower vulnerability. Safer RDX products can be produced in the same manner.

Velocity of detonation of AN base blasting agent with addition of hay and recycled rubber

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Keywords: ammonium nitrate; recycled rubber; hay; detonation velocity.

Commercial Explosives are most often mixtures of oxygen and fuel components and supplements. ANFO explosives and emulsion explosives due to satisfactory detonation properties make the bulk of explosive consumption for blasting in mining industry and open pit excavation in the construction industry. Given the non-explosive properties of the ingredients, they have an advantage over explosive sensitized with nitro-derivatives or monomolecular explosive from the safety point of view. Requirements for the commercial explosives, especially blasting in populated areas, may be contradictory in the sense of the need to create sufficient pressure or mechanical work to fragment the rock, with minimal damage to the surrounding rock, outside the blasting zone and other minimum environmental impacts. By adding organic materials other than conventional explosive components, certain detonation properties may be amplified or reduced, or available energy can be concentrated or impaired in surrounding rock. By using organic waste materials, the detonation properties of the AN mixtures can be adjusted with a satisfactory blasting effect, and the additional benefit of disposal or exploitation of such materials. The paper presents the results of velocity of detonation measurements for the AN mixtures with recycled rubber and hay, in different ratios.

On existence of formic and isocyanic acids in detonation products

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Keywords: detonation products; formic acid; isocyanic acid; EXPLO5; detonation.

Calculation of the composition of detonation products at a given p, V, T condition is a starting point for all thermochemical equilibrium codes that are used for theoretical prediction of detonation properties of explosives. It was reported by many authors that other than main detonation products (such as H2O, H2, CO2, CO, N2, C(s), etc.), some larger uncommon molecules, may also exist in significant amounts and play an important role in the accuracy of thermochemical calculations.

The existence of formic acid (CH2O2) as an important detonation product has been a controversial topic for more than two decades. Kerley (1985) was amongst the first who claimed that formic acid is an important product in the detonation of PETN, RDX and HMX. Baker et al. (2010) and Sućeska et al. (2010) also reported that formic acid is one of the major products formed at higher pressures. Contrary to their findings, Fried et al. concluded that isocyanic acid (HNCO) is a major detonation product for RDX and HMX, but not formic acid. It is obvious that opinion on this issue is still divided.

Since experimental techniques are still unable to reliably measure the composition of detonation products in the reaction zone and at the CJ state, elucidation in this area can only be based on thermochemical and molecular dynamic calculations. In this paper we studied the existence of formic acid and isocyanic acid in detonation products using the thermochemical equilibrium code EXPLO5. We have found that concentrations of formic and isocyanic acids depend on the equations of state of these two compounds, in particular the interaction of potential parameters in EXP-6 fluid equation of state used in the calculations. In any case, experimental detonation parameters for the explosives studied in this work can be reproduced accurately only if formic acid and/or isocyanic acid are taken as major detonation products. Further detailed experimental investigation of the equation of state of these two compounds is called for in order to clarify the existence of formic acid and/or isocyanic acid in detonation products of some explosives.

Effect of polyphenols and ionic liquids as novel stabi-lizers for nitrocellulose

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Keywords: nitrocellulose; polyphenol; ionic liquids; stabilizer; thermal analysis.

Nitrocellulose (NC) spontaneously decomposes even at room temperature, and can ignite because of accumulated reaction heat. To suppress spontaneous decomposition, aromatic amines such as diphenylamine (DPA) are generally used as stabilizers. However, because of the toxicity of these conventional stabilizers, alternative substances have recently been investigated. In this study, we used heat flux calorimetry (C80, SETARAM) to investigate the thermal behavior of NC containing natural polyphenols (ellagic acid (EA), rutin (RU), gallic acid (GA), and resveratrol (RV)), ionic liquids (1-butyl-3-methylimidazolium tetrafluoroborate ([bmim][BF4]), and trihexyl(tetradecyl) phosphonium chloride ([THP][Cl])). We collected measurements under 120 °C isothermal conditions in an oxygen atmosphere, and found that the induction period (tp) for the exothermic decomposition of NC containing polyphenols was longer than that of NC alone, regardless of additive type. This indicates that the investigated polyphenols prevent the thermal decomposition of NC. The stabilization effect order for polyphenols was NC (tp = 4.9 h) < NC/RU (7.7 h) < NC/RV (9.4 h) < NC/GA (9.6 h) < NC/EA (12.4 h). The stabilization effect of polyphenols is not high relative to that of conventional stabilizers (e.g., tp of NC/DPA = 31.9 h). However, the thermal stability of NC could possibly be improved more by the addition of a certain type of polyphenol. In contrast, for ionic liquids, tp was observed to be 3.9–5.6 h, which was approximately the same as or shorter than that of NC alone. Therefore, we do not consider the examined ionic liquids to have exhibited a stabilization effect.

Synthesis of 3,5-diamino-2,4,6-trinitrotoluene via vicarious nucleophilic substitution

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Keywords: 3,5-diamino-2,4,6-trinitrotoluene; vicarious nucleophilic substitution; DATNT; VNS.

The synthesis of the 3,5-diamino-2,4,6-trinitrotoluene (DATNT) by using Vicarious Nucleophilic Substitution (VNS) is presented. Commercial 2,4,6-trinitrotoluene (TNT) was used as a not expensive and convenient substrate. VNS reaction were conducted in DMSO or DMF as a polar and aprotic solvents. Two aminating agents (TMHI, ATA) and three organic bases (MeOK; iPrOK; and t-BuOK) were used. The products were analyzed by using multinuclear NMR spectroscopy and DTA/TG techniques. It has been found that the optimal solvent for the synthesis is DMSO. The raw product is contaminated and requires purification. In this work extraction of DATNT with CHCl3 was used. The product melts at 221 °C and decomposes exothermically with peak maximum at 263 °C (DTA).

Reduction of nitroaromatic explosives by Plasmodium falciparum ferredoxin: NADP+ reductase: estimation of their single-electron reduction potentials

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Keywords: nitroaromatic compounds; ferredoxin: NADP+ reductase; reduction potential.

Single-electron reduction potentials (E1/7) of nitroaromatic compounds are usually obtained by means of pulse radiolysis and flash-photolysis. In the present study we present an alternative method of their estimation, based on the linear log (rate constant) vs. E1/7 dependences in single electron reduction of nitroaromatics by flavoenzymes electrontransferases. The current approach enabled us to characterise the E1/7 values of 10 previously uncharacterized nitroaromatic compounds, including explosives

Energetic polynitrophenyl substituted 1,2,4-triazole derivatives: synthesis, properties and LC-MS analysis

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Keywords: 1,2,4-triazole; nitration; nitrocompound; picrylamino; thermostable; high-energy material; synthesis; LC-MS; flash point.

Synthesis and properties of series of polynitrophenyl substituted 1,2,4-triazole derivatives derivatives are described. Modified, more convenient synthetic methods are based on the condensation reactions supported by microwave activation. The synthesized products were analyzed by LC-MS method. Thermal analysis of selected representatives was done. The most of prepared compounds possess a high melting points (250-320 °C) and exceptional thermal stability, superior to standard HNS, and can find a potential application as thermostable energetic materials. The heat resistant properties of synthesized materials were further confirmed by additional experiments with flash point determination. It was also determined that compounds containing N-NH- fragment, attached to the polynitrophenyl moiety possess decreased thermostability when comparing to the isomeric triazole derivatives, containing in their structure C-NH- fragment. Some calculated preliminary energetic characteristics show that polinitrophenyl substituted triazole derivatives prepared in this work possess a substantially increased energetic properties in comparison with standard TNT. The proposed nitrocompounds may find a potential application as thermostable high energy materials.

Effect of monoammonium phosphate on the thermal stability and detonation characteristics of ammonium nitrate

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Keywords: ammonium nitrate; shock sensitivity; monoammonium phosphate; thermal stability.

A study has examined the effect of Monoammonium phosphate (MAP) on the thermal stability and detonation characteristics of ammonium nitrate (AN). MAP was mixed with AN by two methods. The thermal stability and shock sensitivity of modified AN and ammonium nitrate fuel oil (ANFO) were investigated by differential scanning calorimetry (DSC), the Cook-off test, the Koenen test and UN Gap test. The results show that MAP can increase the thermal stability of AN and ANFO and the water content and mixing methods affected the thermal stability of AN-MAP mixtures. However, ANFO-45wt. % MAP mixtures can still produce a steady detonation in the UN gap test. MAP cannot effectively reduce the shock sensitivity of ANFO. Possible explanations for these results are discussed.

Energetic salts based on 1,2,4,5-dioxadiazine-functionalized nitraminofurazan

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Keywords: energetic salt; dioxadiazine; nitraminofurazan.

Eight nitrogen-rich energetic salts based on the 3,6-bis(4-nitramino-1,2,5-oxadiazol-3-yl)-1,2,4,5-dioxadiazine (H2BNOD) were synthesized and fully characterized by NMR, IR and elemental analysis. Furthermore, H2BNOF (5), ammonium (6),hydroxylammonium (8) and 4-amino-1,2,4-triazolium salts (13) were analyzed by single-crystal X-ray diffraction. The densities of the salts were in the range of 1.730 (13) to 1.914 g cm -3(8).These salts showed much better thermal stabilities and mechanical sensitivities than their precursor, H2BNOD. The decomposition temperatures of the salts ranged from 114 (6) to 197 °C (9). The impact sensitivities of the energetic salts were between 1.5 and 4.5 J, and their friction sensitivities ranged from 53 to >144 N. Their detonation pressures and detonation velocities were calculated to be in the range of 26.3 (12) to 38.1 GPa and 7754 (12) to 9095 m s-1(8), respectively.

Combustion regularities of the propellants on the basis of nitrates of various metals

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Keywords: burning rate; composite propellant; potassium nitrate; sodium nitrate; oxidizer excess ratio.

In this article the regularities of the combustion of high energetic compositions based on potassium and sodium nitrates - were studied. The dependence of burning rate from α for all compositions is extreme. It is shown that the particle size of the oxidant insignificantly affects (from 2% to 10%) the burning rate of the samples. Different catalysts have relatively small effect on the burning rate of high-energetic compositions based on sodium nitrates. The maximum value of Z is observed for copper salicylate.

Energetic salts of pentaerythritol tetranitrocarbamate (PETNC), a PETN analogue

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Keywords: PETNC; polynitro compounds; energetic properties; alcohols.

Starting from the cheap and commercially availably pentaerythritol, the tetravalent pentaeryhtritol tetranitrocarbamate (PETNC) was synthesized in an economic two-step synthesis. PETNC is a suitable starting material for new energetic salts, which were fully characterized using multinuclear NMR spectroscopy, vibrational analysis (IR, Raman), as well as elemental analysis and single crystal X-ray diffraction. The thermal stability was studied using differential scanning calorimetry and the sensitivities against impact, friction and electrostatic discharge were determined. Furthermore, the energies of formation for the nitrogen rich salts were calculated using GAUSSIAN 09. The detonation performances were calculated with the EXPLO5 (V6.03) computer code and compared to pentaerythritol tetranitrate (PETN) and PETNC.

The interaction of 1-ferrocenyl-1,3-butanediol and 1,1'-bisferrocenyl-1,3-butanediol with hexamethylenediamine

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Keywords: ethyl acetate; hexamethylenediamine; glacial acetic acid; ferrocene; ferrocenylbutanediol; ferrocenylbutanetetraol.

The intaraction of 1-ferrocenyl-1,3-butanediol and 1,1'-ferrocenylene-bis-1,3-butanediol with hexamethylenediamine. Characteristics and spectral properties of the hexamethylenediamine derivatives of 1-ferrocenyl-1,3-butanediol and 1,1'-ferrocenylene-bis-1,3-butanediol.

Combustion and explosion characteristics of 5-aminolevulinic acid hydrochloride and its intermediate product

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Keywords: 5-ALA hydrochloride; 5-NLA methyl ester; flammable properties; explosive characteristics.

We investigated the combustion and explosion characteristics of new antitumor drug — 5-aminolevulinic acid (5-ALA) hydrochloride and its intermediate of synthesis — 5-nitrolevulinic acid (5-NLA) methyl ester. The results were obtained by calculations and experimental methods. DSC data obtained at different heating rates and the Kissinger method calculations were used to determinate the kinetic parameters of the thermal decomposition for 5-NLA methyl ester. It was found that 5-NLA methyl ester belongs to a group of substances prone to explosive transformation. The data obtained during experimental period were transferred to the manufacturer — that would help to create a proper explosion protection for work environment and to design technological processes taking into consideration the required precautions.

Laser sensitivity of pyrotechnic compositions

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Keywords: energetic material; pyrotechnic; sensitivity; laser; radiation.

The question of remote initiation of the burning reaction of energy materials, as the way to increase the safety and stability process of initiating reaction, stay actual. The most promising method is the initiation of a combustion reaction by laser. Therefore, the question of the sensitivity of energy materials, in particular pyrotechnics, to laser radiation is arises. Thereby, the sensitivity of pyrotechnic compositions to the action of laser radiation with a power of 1000 mW with a wavelength of 650 nm was investigated.

Energetic formulation based on HMX and eco-friendly polymeric binder

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Keywords: explosives; binders; environment.

In the context of harsher and increasingly complex international and European environmental legislation, numerous states are more and more aware of the necessity for greener munitions development. The aim of this paper is to present some experimental studies regarding a new energetic composition based on HMX and a polymeric binder (based on acrylic acid and ethyl acrylate) which is soluble in water at slight alkaline pH. Furthermore the energetic material recovered has the same physical, chemical and mechanical properties as the raw material.

The kinetic regularities of the heat release in the thermal decomposition of 1,1-diamino-2,2-dinitroethene (FOX-7) and its cyclic homologues

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Keywords: cyclic homologues of FOX-7; single-crystal X-ray ; sublimation; thermal decomposition; kinetics of heat release.

Thermal stability of 1,1-diamino-2,2-dinitroethene (FOX-7), 2-(dinitromethylene)-1,3-diazacyclopentane, 2-(dinitromethylene)-1,3-diazacyclohexane and 2-(dinitro-methylene)-1,3-diazacycloheptane was studied by means of isothermal calorimetry in the temperature range of 160 – 214°C under conditions of continuous evacuation of the system and in the conditions when the ampoules with the sample were sealed under vacuum. The Arrhenius pre-exponential factors and the effective activation energies Ea were obtained. It was shown that the thermal stability of these explosives is significantly different: the FOX-7 is the most thermally stable, 2-(dinitromethylene)-1,3-diazacycloheptane is the least stable compound. The rates of heat release in FOX-7 decomposition in the open system are more than 2 orders of magnitude higher than those in the closed reactor. The kinetics of weight loss in the course of the sublimation of all explosives was studied in the temperature range of 155 – 200°C. The change in the crystal structure of FOX-7 in the course of the sublimation at 60 – 122°C was monitored using single crystal X-ray analysis.

Effect of magnesium hydride (MgH2) on the explosion properties of novel hydrogen-containing metallic composites

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Keywords: novel hydrogen-containing metallic composite; magnesium hydride (MgH2); heat of combustion; minimum ignition energy; minimum ignition temperature.

Novel hydrogen-containing metallic composites based on aluminum, boron, and magnesium hydride are fabricated in a special process. The explosion properties of metallic composites (heat value of combustion, minimum ignition energy and minimum ignition temperature) are studied. The results show that the heat value of combustion and combustion rate of metallic composites are obviously higher than that of aluminum (Al) and boron (B) mixtures. The minimum ignition energies are between 30-100 mJ, which corresponds to the average value of aluminum (Al). The minimum ignition temperature was 440 °C, significantly lower than the minimum ignition temperature of aluminum (Al) 700 °C. Magnesium hydride existing in the metallic composites can change the way of energy releasing and improve the efficiency of energy releasing.

Preparation and characterization of nitraminofurazan-featured composite energetic salts

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Keywords: energetic salt; furazan; energetic material; preparation.

Energetic salts have been the focus in the field of energetic materials. Normally, energetic salts are consisted of a singular kind of cation and anion. We reported here the preparation and characterization of three composite energetic salts which contain two species of cations. The new energetic salts show more comprehensive energetic properties.

Preparation of nano ferric oxide and catalytic performance on thermal decomposition of ammonium perchlorate

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Keywords: ammonium perchlorate; X-ray diffraction; transmission electron microscopy; composite propellant.

A lot of attention has been given to incorporation of Nano-sized oxides including Fe2O3 in ammonium perchlorate (AP) based solid propellants to enhance their final performance. Nano ferric oxide was synthesized by a solid-state reaction method. The obtained products were characterized by transmission electron microscopy (TEM) and X-ray diffraction (XRD) for particle size and purity. Size reduction of the catalyst increases the surface area and hence, the catalytic activity is also increased. The thermal behavior of AP in the presence of Nano-ferric oxide was studied by using differential scanning calorimetriy (DSC). It was found that the average particle size of Nano-ferric oxide prepared was in the range of 30 nm. Interestingly, catalytic activity of AP where the rate of thermal decomposition of AP in the presence of 1% Nano-ferric oxide increased 10% , which have a direct effect on the burning behavior of propellants.

Determination of the purity of CL-20/HMX cocrystals by FT-mir and FT-nir spectroscopy

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Keywords: HMX; CL-20; co-crystallisation; infrared spectroscopy; near IR; mid infrared; PCR.

A new method has been developed for determining the content of free octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) and 2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) in the HMX/RDX cocrystal by Fourier transform infrared spectroscopy (FT-IR), in the regions MIR (mid infrared) and NIR (near infrared) with PCR regression.

Spectral properties of energetic materials and their heating by the near-IR laser

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Keywords: spectroscopy; energetic material; heating; near IR; laser; ignition.

The absorption spectra in the near-IR range for several samples secondary explosives were studied. Heating of explosives of different classes (nitramines, nitro ether, nitroaromatic compounds, C-nitro-NH-azoles, and etc.) by near-IR laser radiation (0.98, 1.55 and 1.94 μm) delivered by optical fiber was studied. The process of laser heating was studied for samples obtained by pressing powdered explosives and for single grown explosives crystals. It was shown that the initial rate of temperature rises at the center of the laser spot when exposed to explosives samples is proportional to the laser radiation power. It has been established that the efficiency of laser heating depends not only on its density, heat capacity and focusing of laser radiation, but also on the scattering properties of the material. It has been shown that the efficiency of laser heating for pressed explosives samples is 2-5 times greater than the efficiency for samples in the form of an individual crystal. It is shown that the efficiency of laser heating for compounds containing N-H bonds at wavelengths of 1.56 μm to 50-100 times higher than at 1.94 and 0.98 μm. The reported study was funded by RFBR according to the research project No 16-29-01072 ofi-m.

The cation-radical step in the nitration of 2-alkyl-substituted 4,6-dioxopyrimidines

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Keywords: cation-radical; EPR; UV-spectroscopy; nitration; 4,6-dioxopyrimidines.

Electronic paramagnetic resonance and ultraviolet spectroscopy have shown the formation of cation-radical by nitration of alkyl-substituted 4,6-dioxopyrimidines. The kinetics of formation of cation-radical and their transformation into a sigma-complex is studied. The composition of the conversion products of the cation-radical was determined.

Synthesis and reactivity of nitro- and nitroso-derivatives of 6-hydroxy-2-methylpyrimidine-4(3H)-one

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Keywords: 6-hydroxy-2-methylpyrimidine-4(3H)-one; kinetic; nitration; nitrosation; nitrogen oxides.

The nitration reaction of 6-hydroxy-2-methylpyrimidine-4(3H)-one in a medium of 72-82% sulphuric acid was studied. The nitrogen oxides influence on this process was discovered. New nitro- and nitroso-derivatives of 6-hydroxy-2-methylpyrimidine-4(3H)-one were synthesized.

Characterization and optimalization of electrostatic discharge (ESD) sensitiveness of potassium 4,6-dinitrobenzofuroxane

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Keywords: ESD; KDNBF; potassium; 4,6-dinitrobenzofuroxane.

It was found that the electrostatic discharge sensitivity of potassium 4,6- dinitrobenzofuroxane (KDNBF) have risky value of minimal initiation energy (MIE) value. The lowest measured energy was within the range of 30 μJ. Additions of conductive graphite to KDNBF didn't changed MIE level significantly. Efforts has been made to find way how the graphite addition influence ESD sensitiveness in form of threshold initiation level and probability of sample initiation. It was found that the MIE values remains still but conductive admixtures influenced the probabilities of initiation. The highest measured energy without initiation of sample changed with the content of graphite. Influence of ultrasonic homogenizers on MIE levels was studied.

Photochemistry of metal oxide – energetic material interfaces

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Keywords: photochemistry; optical initiation; organic-inorganic interface; spectroscopy.

Organic–inorganic interfaces provide both intrigues and opportunities for designing systems that possess properties and functionalities inaccessible by each individual component. The report is devoted to theoretical and experimental research of metal oxide – energy material interfaces optical properties. Aluminum and magnesium oxides, rutile (titanium oxide), pentaerythritol tetranitrate (PETN) and trinitrotoluene (TNT) were used as the objects of the study. The processes of photoinduced charge transfer in interfaces and the possibility of the photocatalytic decomposition reaction of the energetic material are considered. The fundamental conditions and limitations of the metal oxides application as a photocatalytic sensitizing additive during the optical initiation of energy materials are formulated.

Keyword Index

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The End