Abstracts of the 22nd Seminar on

New Trends in Research of Energetic Materials

NTREM

Pardubice, April 10–12, 2019

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

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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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Part 2

Preface

Over the last few years University of Pardubice has gained certain dynamism and ability to develop rapidly, including the construction of a bilingual environment. This development, including the activities of the University in the field of international relations in science and education, has a synergy positive effect on the implementation of the NTREM International Seminars. It is well known that our Seminars serve mainly to the young scientists and students in their orientation and study of the Science of Energetic Materials, scooping needed to mention also the numerous quotations in the scientific literature of the papers presented on these meetings. However, the original way of the organization of these meetings was marked by the great uncertainty of the participation of the authors who registered and in some case also sent full texts of their contributions and then did not attend. This uncertainty caused a big problem in the confection of both the lecture and poster programs and therefore, starting with this 22nd seminar, registration fees and review of registered abstracts by the Scientific Committee were introduced. The introduction of the review process resulted in an earlier deadlines for abstract as well as full text submissions. This could have been a surprise for those interested in attending this meeting; however as it seems today, most of the contributing authors and participants mastered this change very well. A great work, related with this new organization and preparation of this year's meeting, has been done traditionally by our organizing committee under leadership of Assoc. Prof. Jiri Pachman with members of this committee, especially treasurer Dr. Marcela Jungová, co-editor of the proceedings, Dr. Šelešovský and representative of Dean's office, Dr. Iva Ulbrichová; thanks a lot for their perfect organization and services.

The registration fee introduced this year aimed at elimination of unserious contributions on one hand while not limiting attendance of young participants on the other. As such it was set to the level which is not able to cover the cost of the seminar and we have to rely on our traditional supporters. The Seminar is 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. The organisation of the 22nd NTREM in 2019 was made possible thanks to the following supporters:

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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.

And traditionally, let mi thank 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 goodbye till next April.

Pardubice, February 28th, 2019

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Development of promoters for hypergolic reactions

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Keywords: ionic liquid; hypergolic propulsion; 3-ethyl-1-methyl-1H-imidazol-3-ium cyanotrihydroborate; iodocuprate-containing ionic liquids.

Many Energetic Ionic Liquids (EILs) were reported as promising hydrazine-replacement fuels for hypergolic rocket propulsion. However, many of these EILs were ignited by corrosive and hazardous concentrated fuming nitric acid. Significant efforts were recently made to utilize highly-concentrated H2O2 as a "green" alternative to fuming nitric acid and N2O4 oxidizers. Although "rocket grade" H2O2 is more challenging for use and less safe for storage than commercially-available H2O2 (70%), the latter was not considered as a viable oxidizer for hypergolic propulsion. In our work, we focused on the development of novel iodine-rich promoters, capable to initiate hypergolic ignition reactions between a typical EIL fuel – 3-ethyl-1-methyl-1H-imidazol-3-ium cyanotrihydroborate and H2O2. Among prepared and evaluated promoters, the top performing [FcCH2NEtMe2+]2[B12I122–] showed ignition delay times of 45 msec in reaction of the tested EIL with H2O2 (70%) and 17 msec with H2O2 (95%). We also developed four novel iodocuprate-containing ionic liquids (CuILs), which exhibited capability to efficiently promote hypergolic reactions between EIL fuels and highly-concentrated H2O2. The most promising promoter of CuIL type has high decomposition temperature, was found to be stable in promoter-in-fuel formulation for weeks and showed ignition delay times of 14 msec. We believe that our findings provide a platform for the development and utilization of H2O2 as potential "green" oxidizer for space propulsion.

Synthesis of melt-castable explosive and propellant plasticizing materials

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Keywords: energetic material; synthesis; explosive; propellant.

Given the environmental and toxicity concerns associated with TNT, and the low performance values of DNAN-based formulations that have replaced TNT, there is an interest in the development of new melt-castable explosive ingredients that possess both low toxicities and high detonation characteristics. From the aspect of propellant ingredients, while much attention has been paid to the synthesis of new CHNO-based oxidizers, the development of new energetic plasticizer materials has received much less attention. Yet such ingredients, in an effort to extend the range of propellant munitions, are needed in an effort to potentially replace the inert plasticizers currently in use. Discussed will be the synthesis of several melt-castable (both standalone and eutectic) and energetic plasticizer materials for potential explosive and propellant formulation applications. Presented will also be the sensitivities, performances, experimentally determined densities, and where applicable, the development of new synthetic methodologies in making the explosive and propellant ingredients.

Prediction of high energy molecules properties using recursive molecular search (R.Mo.S)

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Keywords: prediction; toxicology; physico-chemistry.

Since 2007, European regulation REACh (Registration, Evaluation, Authorization and restriction of Chemicals) places responsibility on industry to manage the risk from chemicals and doing so, to ensure a high level of protection of human health and environment. In line with these restrictions, Ariane Group has set up a collaborative project with the CNRS (French National Center of Scientific Research) intending to develop optimized tools to predict High Energy Materials (HEM) properties, such a as toxicity. All these prediction tools would be involved in a rational design strategy called the Toolbox Program.

Several in silico methods can be used to predict properties of molecules, such as QSAR, Local QSAR, or Machine Learning. We have already demonstrated that using Local QSAR allows a better prediction and a good reliability1. To perform this kind of prediction, a subset of molecules must be set from a large database. Afterward, the classical approach is to compute the similarity distance between the molecule to be predicted and the database. Molecules are then selected or not, depending on a distances value cutoff.

We develop here a new approach called Recursive Molecular Similarity (R.Mo.S). The algorithm computes the similarity distance between the molecule to be predicted and all other molecules. Then the algorithm determines a virtual signature molecule. This signature molecule is later used to compute the similarity distance with all previously unselected molecules. This calculation is repeated iteratively until there are no new molecules to put in the subset, or the determined number of recursive iterations is reached.

This presentation focuses on applications of prediction of physical properties, such as the boiling point for HEM. It also focuses on toxicological prediction, in agreement with REACh. This legislation describes the international guidelines of the different toxicological tests. Databases used in this study compiled available data on mutagenicity, carcinogenicity and reprotoxicity for a broad spectrum of molecules. Regarding the boiling point, the database was extracted from the Reaxys database with a pressure of 1 atm.

This prediction tool will be compared with softwares often used in the scientific community such as ACD or ChemAxon.

1. Alliod et al. Propellants, Explosives, Pyrotechnics. 2017, 42,1, 24-35.

Characterizing of glass-rubber transition shift in filled HTPB-IPDI formulations by modified and normal Arrhenius equation

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Keywords: HTBP-IPDI formulations; glass-rubber transition shift; modified Arrhenius equation; WLF equation; normal Arrhenius equation.

The glass-rubber transition (GRT) in elastomer bonded energetic material as composite rocket propellants and high explosives is an important property for the use of these materials. The temperature range of application of such rubber materials is always above the GRT, in contrast to thermoplastic elastomers, which are used below the GRT. The GRT is strongly determined by intermolecular interactions. An important behaviour is the deformation rate dependence of the GRT. With increasing deformation rate, means measurement frequency in dynamic mechanical measurements, for example, the GRT is shifted to higher temperatures, means the in-service temperature range changes. The interaction between the binder polymer chains surely changes with the type of solid filler, as RDX or AP (ammonium perchlorate). Based on recent work using HTPB-IPDI (hydroxyl-terminated polybutadiene-isophorone diisocyanate) polyurethane binder, the determined data on GRT shifts are re-characterized by the so-called modified Arrhenius equation (MAE), which has proven to be equivalent to the WLF (Williams-Landel-Ferry) equation. The MAE has some advantages against WLF: no data are lost by setting a reference Point out of measured data and the WLF invariant C1C2 is expressed with an activation energy, which is used to interpret interaction in the material. A comparison with the activation energies obtained with the normal Arrhenius equation (NAE) is made.

Lithium dihydrobis(azolyl)borates as colorants for strontium- and chlorine-free red pyrotechnics

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Keywords: lithium dihydrobis(azolyl)borates; red pyrotechnic colorants; environmental friendliness.

In 2014, the U.S. Environmental Protection Agency declared strontium to be harmful to health based on findings of its adverse effect on the human bone strength with calcium deficiency and during skeletal development. When this contaminant was determined to be present in 99% of all public water systems in the U.S. and in 7% out of these even at levels of concern, the EPA was considering to regulate the amount of strontium in drinking water. While the potential carcinogenicity of polychlorinated aromatics, released during the combustion of chlorinated material, had long been known at this point, this recent progress again revolutionized the way of producing red light in pyrotechnics. This work approaches the current issue of banning both chlorine and strontium from pyrotechnic formulations by proposing lithium dihydrobis(azolyl)borate salts as alternative colorants which generate metastable atomic lithium as the red light-emitting species in the flame. Such moieties should not only be environmentally benign in terms of their emitter but also in regard of their combustion products. The driving force for an efficient burn-down is the formation of molecular nitrogen and diboron trioxide. Detailed information are given on the synthesis of the lithium salts of dihydrobis(pyrazolyl)borate, dihydrobis(1,2,4-triazolyl)borate and dihydrobis(1H-tetrazolyl)borate as well as on the analytics and on their optical performance in pyrotechnic compositions.

Study on the structure-property relationship of energetic metal-organic frameworks: A guide to the development of high energetic materials

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Keywords: metal-organic framework; structure-property relationship; energetic materials.

The study of structure-property relationship is one of the key pillars of energetic materials since it would allow for better design and achievement of desired properties. Here two kinds of energetic metal-organic frameworks (MOFs): 3D cationic MOFs (CMOFs) and 1D neutral MOFs (NMOFs) using two different ligands 4,4'-bi-1,2,4-triazole (btrz) and 4,4'-azo-1,2,4-triazole (atrz) were synthesized and characterized. For the 3D cationic MOFs, the effect of ligand backbones and anionic groups were studied, and the results showed that the effect of ligand backbones on the CMOFs is inverse that of the backbones on traditional energetic compounds, while the effect of the anionic groups follows the traditional group law. In addition, for the 1D NMOFs, [Cu(btrz)2(DNP)2, DNP=3,5-dinitropyrazolate anion] has higher density than its analogy [Cu(atrz)2(DNP)2], although ligand atrz has higher density. This investigation of understanding the structure-property relationship in energetic MOFs will bring about new insight for the design and synthesis of novel high energetic materials.

Synthesis and characterisation of tri- and tetraethyleneglycoldiazide for their use as energetic plasticisers

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Keywords: synthesis; characterisation; energetic plasticisers; triethyleneglycoldiazide; tetraethyleneglycoldiazide.

Tri- and tetraethyleneglycoldiazide (TEGDA and 4EGDA) were synthesized from their corresponding chlorides by a reaction with sodium azide in water with a phase transfer catalyst in batches up to one kilogram of the product. The influence of the plasticisers on the glass transition temperature of different glycidyl azide polymer (GAP) formulations was evaluated by differential scanning calorimetry (DSC). Their compatibility to different fillers was evaluated by heat flow calorimetry (HFC). The solubility of ammonium dinitramide (ADN) in the plasticisers was also measured.

Using natural language processing techniques to extract information on the properties and functionalities of energetic materials from large text corpora

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Keywords: natural language processing; machine learning; formulations; energetic materials.

The number of scientific journal articles and reports being published about energetic materials every year is growing exponentially, and therefore extracting relevant information and actionable insights from the latest research is becoming a considerable challenge. In this work we explore how techniques from natural language processing and machine learning can be used to automatically extract chemical insights from large collections of documents. We first describe how to download and process documents from a variety of sources - journal articles, conference proceedings (including NTREM), the US Patent & Trademark Office, and the Defense Technical Information Archive on archive.org. We present a custom NLP pipeline which uses open source NLP tools to identify the names of chemical compounds and relates them to function words (“underwater”, “rocket’”, “pyrotechnic”) and property words (“elastomer”, “non-toxic”). Relationships are obtained by doing computations with word vectors. After explaining how word embeddings work we compare the utility of two popular word embeddings - word2vec and GloVe. We show that word embeddings capture latent information about energetic materials, so that related materials appear close together in the word embedding space. Analytics on common compounds and topics for NTREM and other proceedings and how they have changed with time are also presented.

New family of energetic salts incorporating tetrazolylfuroxan core

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Keywords: 1,2,5-oxadiazole 2-oxide; furoxan; tetrazole; energetic salts.

A new family of energetic salts with high nitrogen content comprised of the tetrazolylfuroxan core and explosophoric azido and azo groups has been synthesized through a three-step procedure from readily available furoxancarbonitriles. This approach involves [3+2] cycloaddition of an azide-anion to the corresponding furoxancarbonitriles with subsequent double cation metathesis. The structure of all newly synthesized high-energy salts was confirmed by 1H, 13C, 14N, 15N NMR and IR spectroscopy and X-ray diffraction studies. Densities, thermal stability, impact and friction sensitivities of all compounds were determined. Enthalpies of formation and detonation parameters (detonation velocity and pressure) were calculated. According to our results, several synthesized compounds have good densities, high thermal stability and high enthalpies of formation and may serve as promising ingredients for high-energy formulations.

4,4‘-Bipyrazole as a building block for new energetic materials

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Keywords: energetic materials; polynitro azoles; structure elucidation; high explosives; N-functionalization of bipyrazoles.

Nitrogen-rich heterocycles play an important role as building blocks in the development of new high energy density materials, (HEDMs). For the past 20 years scientists have investigated different five- and six-membered heterocyclic systems (e.g. azoles, triazines, diazines and tetrazines) as potential new high explosives. 3,4,5-Trinitropyrazole, 4,4‘,5,5‘-tetranitro-bisimidazole and 4,4‘,5,5‘-tetranitro-bipyrazole are prominent examples for azole based explosives which exhibit not only good stability toward external stimuli but also show high performance. Theoretical calculations have shown that polynitrated 4,4‘-bipyrazole explosives may exhibit even better performance than the literature known explosives. In this study we present the scaffold functionalization of 3,3‘,5-trinitro-4,4‘-bipyrazole and 3,3‘,5,5‘-tetranitro-4,4‘-bipyrazole. The new polynitro azole based explosives were characterized by means of multinuclear (1H, 13C, 14N) NMR spectroscopy, mass spectrometry, vibrational spectroscopy (IR and Raman), elemental analysis, DTA measurements and by low-temperature single-crystal X-ray diffraction. In addition, the sensitivities of the new synthesized polynitro azoles toward impact and friction were tested according the BAM standards.

Nitro derivatives of benzo[c]cinnoline-5-oxide as new energetic compounds

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Keywords: nitration; heat resistant explosives; NMR spectroscopy; thermal properties.

Benzo[c]cinnoline-5-oxide (BCO) was obtained via reduction of 2,2'-dinitrobiphenyl by basic solution of sodium sulphide. BCO was purified by crystallization from aqueous ethanol. Nitration mixtures with different coefficient of nitration activity were used. Four nitro derivatives were obtained (2-nitrobenzo[c]cinnoline-5-oxide, 2,4,8-trinitrobenzo[c]cinnoline-6-oxide, 2,4,10-trinitrobenzo[c]cinnoline-6-oxide and 1,3,7,9-tetranitrobenzo[c]cinnoline-5-oxide). Products were separated in laboratory scale by column chromatography. Benzo[c]cinnoline-5-oxide and its nitration products were analyzed by multinuclear NMR spectroscopy (1H, 13C, 15N). Thermal properties and stability determined by thermal analysis were compared to commonly known energetic nitroaromatic compounds. Tetranitro-BCO undergoes exothermic decomposition over 300°C and can be considered as new interesting energetic compound for special applications.

Studies of the ballistic parameters of new complex propellants

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Keywords: propellant; heat of combustion; combustion pressure; thermochemical calculation.

New complex propellants based on RDX were obtained and investigated. Heats of combustion were determined in a calorimeter and pressures histories were measured in a manometric bomb. Such ballistic parameters as maximum pressure, propellant force and covolumen of gaseous products were determined based on the experimental results. Sensitivities to friction and impact were determined for the tested propellants. The calculations of the ballistic parameters (the heat of combustion, propellant force, covolumen and ratio of specific heat of combustion products, and ballistic energy) were performed using the CHEETAH code. The theoretical parameters were compared with the experimental data. The analysis of test results and the comparison of the parameters of complex propellants with the parameters obtained for the JA-2 propellant allowed to assess the possibility of using the tested propellants in ammunition.

Combination high energy with stability: polynitrogen explosives N14 and N18

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Keywords: N14; N18; density functional theory (DFT); high energy; stability.

High energy density materials (HEDMs), which possess not only perfect detonation performance but also good thermal stability and low sensitivity, have attracted considerable interests for some potential applications in propellants, explosives and pyrotechnic agents in recent years. Two novel high energy density materials N14 (1,6-dihydro-1,2,3,3a,4,5,5a,6,7,8,8a,9,10,10a-tetradecazapyrene) and N18 (1,2,2a,3,4,4a,5,6,6a,7,8,8a,9,10,10a,11,12a-octadecazacoronene) were designed, and their structures, detonation performances and stabilities were calculated employing density functional theory (DFT). In high energy density materials, the crystal density (ρ) is an important parameter for predicting performance. Their densities are 1.784 and 1.817 g/cm^3, respectively. As these two compounds contain mainly C and N, and don‘t contain O, their densities are lower than HMX and CL-20. The isodesmic reactions were used to predict the heat of formation (HOF) of compounds. The HOFs of N14 and N18 are 2142.17 and 2959.60 kJ/mol, respectively. Due to lots of nitrogen which are connected directly, the values are much higher than RDX, HMX or CL-20. Detonation performances were estimated using EXPLO 5 (v6.01) and calculations reveal that they two have an excellent power. Detonation performance of the N14 (P = 43.6 GPa, D = 10040 m/s, Q = 2214 cal/g) and the N18 (P = 37.4 GPa, D = 9400 m/s, Q = 2114 cal/g) are comparable to CL-20 (P=44.1 GPa, D=9380 m/s, Q=1567 cal/g). This paper also presents electrostatic potential maps, impact sensitivities, and energy gaps between LUMO and HOMO orbitals. Considering their excellent detonation properties, they are all likely to be used as candidates of high energy density materials. Further work on route optimization and practical synthesis is being carried out by our team.

Preparation and dismantlability evaluation of urethane acrylate resin containing inorganic salts

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Keywords: dismantlable resin; tensile test; nitrate; perchlorate; iodate.

A dismantlable adhesive is a kind of the eco-friendly material that can easily lose the adhesion strength by external stimuli like heating, which can facilitate recycling materials bonded with adhesives. The previous study revealed that oxidative or halogen-containing inorganic salts can act as effective additives to give dismantlability to epoxy adhesive. In this study, in order to develop the different type of the dismantlable resin, the mixtures of urethane acrylate resin (UA) and an inorganic salt (NH4ClO4, NH4NO3, NH4IO3, or NH4Cl) were prepared, and their dismantlability after heating was evaluated using the tensile test. The results showed that the tensile strength of all of the prepared UA decreased after heating at 200 °C compared to that without heating, although no change was observed at 150°C or less. Since the strength of UA alone did not change at 200 °C, the addition of the inorganic salts is thought to be effective to give UA dismantlability. From further investigation on different heating conditions and addition amounts, it was ultimately considered that the order of the effect decreasing the tensile strength is NH4NO3 » NH4IO3 > NH4Cl ≈ NH4ClO4. The melting points of NH4NO3 and NH4IO3 were less than 200 °C that is lower than that of NH4ClO4, suggesting that melted salts or decomposition products react with UA to decrease the strength, and oxidative inorganic salts having a low melting point is suitable as an additive for dismantlable UA.

Dependence of the specific impulse of solid composite propellants basing on oxidizers with NF2-groups on aluminum content in the formulation

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Keywords: propellant; NF2-containing oxidizer; aluminum; specific impulse; combustion products.

Earlier it was shown that in metal-free propellants based on difluoramines as oxidizers the maximal values of specific impulse are achieved at the ratio F/H=1. In the investigation under consideration it is shown that if the compositions contains Al additives the maximal values of specific impulse are achieved at the ratio F/H>1. A thorough study of the dependence of Isp and the combustion products upon the content of aluminum, fluorine, etc. allowed us to find a new pattern — in the presence of aluminum the optimal F/H ratio for the highest Isp values achievement increases until at the exit nozzle section COF2 begins to form. It has been specifically shown that this is due to the fact that after all hydrogen has been oxidized by fluorine to HF, the remaining amount of fluorine (at F/H> 1) leads to the formation of gaseous fluorides (mainly AlF3) and aluminum fluoroxides with significantly larger thermal effect than the carbon oxidation into COF2 may provide.

Mesoscale simulation of shock ignition in PBX explosives

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Keywords: explosion mechanics; heterogeneous explosives; mesoscale structure; shock loading.

To investigate the mechanism of shock ignition in heterogeneous explosives, mesoscale simulation of PBX explosives under shock loading was conducted. Through simulation of explosive particles pressing, mesoscale structure of PBX was obtained. Then the shock ignition of PBX explosives was calculated, and the coupled thermo-mechanics and self-heating reaction were considered, and the influence of explosive density, particle size and binder content on shock ignition were analyzed. The results show that hot spots focus on the interface between explosive particles and binder. The critical pressure of explosives in small particle size is higher than that in large particle size. The critical pressure of explosives in low density is higher than that of explosives in high density. In addition, binders play an important role in attenuating shock compression on explosive particles, and PBX explosives in high binder content are more insensitive than those in low binder content.

Electrospinning preparation of micro/nanoscale-Al/MoO3 thermite fibers with enhanced combustion performances through incorporating nano-carbon materials

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Keywords: electrospinning; thermite; combustion performance; heat transfer coefficient.

The combustion performance of thermites relies on many parameters, such as their heat transfer efficiency and the activity of the metals. Nano-carbon materials are well-known for their superior heat transfer behavior. And a versatile way to maintain the activity of the metals is to cover them with another inert material. Electrospinning technique is capable of covering the particles with organic fibers to maintain the activity of the metals. In order to enhance the combustion performance of Al/MoO_3 thermite, as well as protect the activity of aluminum, three different kinds of nano-carbon materials were incorporated into the formulations by means of electrospinning technique with nitrocellulose as the carrier. Three scale levels of aluminum particles, i.e. micro-, sub-micro- and nano-aluminum, were used in the formulations. Morphologies, elements distributions, phase structures and heat transfer coefficients of the samples were analyzed by scanning electron microscope (SEM), energy dispersive spectroscopy (EDS), X-ray diffractometer (XRD) and heat flow meter, respectively. XRD and EDS measurements confirmed the existence of all ingredients. SEM results proved that electrospinning technique is an efficient mean of uniformly distributing all ingredients in general. Heat flow meter results showed that the raw thermites fiber, nano-Al/MoO_3 in particular, gained better heat transfer performances with the addition of nano-carbon materials especially reduced graphene oxide. As for combustion performance, nano-Al/MoO_3 fiber owned highest combustion rate of all, while nano-carbon materials were most helpful in elevating the combustion rate of sub-micro counterpart. Among three kinds of nano-carbon materilas, reduced graphene oxide was the most efficient one in enhancing combustion rates of samples. Overall, the addition of nano-carbon materials into thermite formulation can efficiently increase the combustion as well as heat transfer performance of micro/nanoscale-Al/MoO_3 thermite fibers.

Investigation of detonation properties of tetranitromethane/methanol mixture

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Keywords: detonation; liquid high explosives; tetranitromethane.

The chemical reaction in shock-condensed liquid high explosives (HE) has a thermal character, and initial rate of reaction is a strong function of activation energy. It can change in a wide range by addition of diluents to HE. Definition of the initial rate value gives important information for prediction of HE detonation due to its influence on the detonation wave structure and propagation limits. In this work, the reaction zone structure, stability of detonation waves and limits of detonation propagation in the mixture of tetranitromethane/methanol (TNM/M), depending on the diluent concentration, were investigated by VISAR interferometer. In the experiments, TNM with 1.64 g/cc initial density and 6.4 km/s detonation velocity and methanol with 0.79 g/cc initial density were used. On the dependence of particle velocity on time, in the neat TNM behind the shock jump the velocity decreases smoothly and the maximum velocity gradient is realized directly behind the shock wave front. At the addition of methanol to TNM, the amplitude of Von Neumann spike begins to decrease, whereas detonation parameters increase. At the methanol concentration of 15-35%, there is a sharp change in the character of the reaction zone – after the initial shock jump, the particle velocity continues to increase, for approximately 10 ns, reaches maximum, and then drops. At further increase of methanol concentration to the critical concentration of detonation (60%), the detonation parameters decrease and oscillations appear on the velocity profiles. It means that detonation front becomes unstable. The dependence of detonation velocity of the mixture on methanol concentration is non-monotonically. The maximum value of detonation velocity is observed at a small negative oxygen balance (26-28% of methanol). The thermodynamic calculation with the BKW-RR equation of state agrees well with the experimental data and reproduces the discrepancy between the maximum detonation velocity and the stoichiometric concentration of the mixture. This work was supported by Russian Foundation for Basic Research (project No.16-29-01002).

Influence of reaction rate on optical emission spectra of HMX

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Keywords: optical spectroscopy; deflagration; detonation; HMX.

The optical emission spectra of energetic materials (HMX, RDX, PETN) during the three regimes of burning, deflagration and detonation were studied. Detonation of a column of pressed granulated HMX at 80 percent TMD was achieved, with the detonation front velocity measured at 7.8 km/s. The main spectral emission was from alkali metal impurities, in particular the sodium doublet at 589 nm. The broadening and redshift of this peak with higher reaction temperatures and pressures were measured, as well as the competing blackbody emission. Temperatures were calculated from the spectra, with deflagration at 4000 – 5000 K and detonation at 7000 K. The higher figure is likely due to the higher pressure detonation adiabatically compressing interstitial gases to temperatures greater than those associated with the chemical reactions alone.

Study on explosive properties of BCHMX

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Keywords: BCHMX; explosive properties; detonation.

A bicyclic nitramine cis-1,3,4,6-tetranitrooctahydroimidazo-[4,5-d]imidazole (bicyclo-HMX, BCHMX) is an energetic material with a heat of explosion and a relative explosive strength exceeding that of β-HMX. Although a lot of research was done to study the performance of compositions with different explosives and to analyse the effect of various polymeric matrices, there is a lack of reported explosive properties of BCHMX in the literature. In order to change that, the material was synthesized from easily available substrates, recrystallized, and flegmatized with Viton. The morphology of crystals was studied with optical microscopy. Afterwards, it was pressed and used in a form of cylindrical charges. Amongst the test methods which were applied in the study, we can name the determination of blast wave parameters, critical diameter, and the gap test. The experiments were also done for flegmatized RDX and HMX and the results were compared.

Crystal engineering of energetic materials: Co-crystal of 2,4,6-trinitrophenol with modified performance and improved sensitivity

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Keywords: picric acid; sensitivity; co-crystallization; safety; energetic materials.

This paper discusses the molecular structures and intermolecular interactions of pure Picric Acid and Picric acid-based energetic-non energetic co-crystals. We find that picric acid co-crystals arrange in layered motifs, while pure Picric Acid features irregular, herringbone packing. Overall, the non-covalent interactions govern the structures of the co-crystals. The results showed that π-stacked structures in explosives, particularly planar layers, are very helpful to decrease their impact sensitivities and to enhance their molecular stabilities. The physicochemical properties of the compounds are theoretically and experimentally investigated in detail. Formation of enthalpy, the optimized structures, molecular total energies, frontier orbit energies, and charge densities of cocrystals are calculated by theoretical methods. These results confirm that a layered packing and strong hydrogen bonding are among the key factors for insensitive co-crystal explosives. The co-crystals sensitivity was found to be about 50% less impact sensitive than Picric Acid, all of which illustrate how co-crystallizations can be utilized for successfully modifying specific aspects of energetic materials.

Influence of ballistic modifiers on the combustion wave of low-calorie propellant

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Keywords: burning rate; double base propellant; flame structure; combustion wave; combustion temperature.

The effect of a combined ballistic modifierconsisting of organic nickel salt and carbon materials, such as carbon black and multi-walled carbon nanotubes, on the burning rate of low-calorie propellant, and on parameters of the combustion wave, such as combustion surface temperature, temperature gradient, and burning temperature, have been studied. Condensed phase heat balance is compiled. The surface structure of quenced propellant with carbon materials, ballistic modifier and its combination is studied.

Design and fabrication of aluminum-free energetic thermites films with high activity, energy density and stability

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Keywords: metal-organic framework; energetic materials; electrostatic spinning; ignition capability.

Energetic thermites films have been widely used in the field of microscale energy-demanding systems because these materials can release a large amount of stored energy on combustion. Even though aluminum-based films have been studied for years, developing novel, facile, and scalable methods to synthesize energetic films with high-energy-density and high stability is still a persistent challenge. Here, we report a new concept aluminum-free thermites based on an energetic metal-organic framework [Cu(atrz)3(NO3)2]n (MOF(Cu), atrz = 4,4′-azo-1,2,4-triazole) as a fuel through the electrostatic spinning method for the first time. Compared with the traditional aluminum-based thermites films, this new films exhibit superior performances such as low electrostatic discharge sensitivities, low ignition temperatures, high heats of reaction, high activity, and production of very few solid residues. It is anticipated that this work will open a new field for the application of MOFs for energetic thermites films, while laying the groundwork for the development of new energetic materials.

Detonation reaction zone in nitromethane: Experimental and numerical studies

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Keywords: nitromethane; reaction zone; Doppler velocimetry; numerical modeling.

The detonation reaction zone in nitromethane (NM) sensitised with 1% of ethylene diamine (EDA) and mixture of nitromethane and 10 % EDA is studied experimentally and by numerical modelling. The experiments involved measuring of the particle velocity history using impedance window technique instrumented with photonic Doppler velocimetry. The diagnostics allow to partially resolve the reaction zone profile. Numerical modelling was done by EXPLO5 thermochemical code using its kinetic detonation module. The module includes slightly divergent Wood-Kirkwood detonation theory and the pressure-dependent reaction rate model, and it enables modelling of time dependent phenomena in the detonation reaction zone. The measured particle velocity profiles of nitromethane agree with the ZND theory: A sharp spike followed by rapid drop in particle velocity over first 25 ns, and then a slower decrease toward the CJ point, which is reached after 55 ns for NM, and 77 ns for NM/EDA. The measured CJ pressure of NM (12.6 GPa) and detonation velocity (6300 m/s) agree well with the literature reported values. The reaction rate parameters are calibrated on the basis of experimentally obtained particle velocity profiles. Using so obtained kinetic parameters, time distribution of parameters within detonation driving zone (including flow parameters, fraction of unreacted explosive, concentration of individual products, thermodynamic parameters of unreacted explosive and reaction products, pressure, temperature, density, etc.) is calculated starting from the von Neumman spike down to the sonic point. A good agreement between experimental and calculated detonation velocities and particle velocity and pressure profiles is obtained.

Development of inert simulants for high explosives at the JRC Geel – problems and perspectives

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Keywords: simulant; aviation; security; terrorism; explosives.

This paper describes the development of polymer-bonded simulants intended to be used as European standards for verifying the performance of explosive detection systems (EDS) used in civil aviation to screen hold baggage. There are around one billion air passengers each year in the European Union, and European legislation requires that each item of hold baggage is screened for prohibited items before being loaded onto the aircraft. In most cases, this screening is done with dual-energy, x-ray equipment with automated detection of explosives. In aviation security, this equipment is referred to as explosives detection systems (EDS). Although such equipment is extensively tested before approval by EU Member States, there are limited means to verify the continued performance of the equipment after it has been installed in airports, due to the impracticality of using energetic materials in an airport, and also because the specific performance requirements are classified. For this reason, we have developed a range of explosives simulants, covering different categories of materials. This paper describes the challenges in developing, producing and validating simulants, in order to provide the necessary quality assurance and quality control for use in routine testing and formal inspections. Topics such as measurement precision, calibration, validation with real energetic materials, material processing, and stability are discussed. We will also report on our latest work to dope our simulants with actual energetic materials synthesised in-house, to produce next-generation, dual-purpose simulants that can be used to check both EDS and trace detection equipment (via swabbing of the material).

A novel energetic nanomaterial based on nanoporous carbons

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Keywords: nanoporous energetic material ; energetic nanomaterial ; activated carbon; nanoporous carbon.

The well-developed three-dimensional porous network of nanoporous carbon, especially in the nanometer range, confers to this material a very high porosity whereas, at the same time, it exhibits excellent mechanical properties [1,2]. This work investigates the potential use of nanoporous carbon as a fuel matrix for composite energetic nanomaterials, where the porous structure is filled with an oxidizing agent and the mechanical properties are provided by the carbon skeleton itself. This novel energetic nanomaterial is expected to combine the promising features of a nanoscale mixture, an oxygen balance close to zero and a very high density (close to or even higher than 2 g/cm^3) while avoiding the obstacles which have hampered the progress toward large-scale practical application of other energetic nanomaterials like very expensive synthesis processes or health and environmental issues.

In contrast with nanoporous silicon filled with an oxidizing agent which has been recently studied as an energetic nanomaterial [3] but can only be synthetized as micrometer-thick layer, nanoporous carbon is a versatile three-dimensional material which has been used as separation media for centuries and has been extensively studied and described in the literature for decades [2]. Nanoporous carbon is nowadays produced at industrial-scale and can easily be shaped, notably by extruding or pressing. Furthermore, it has been shown that the use of carbon nanomaterials in energetic compositions can greatly improve their thermal stability and sensitivity [4] and those benefits are likely to be provided by nanoporous carbon as well. Its textural properties and surface chemistry can moreover be finely tuned to the application, allowing energetic nanomaterials based on nanoporous carbon to be investigated as insensitive and high-performance propellant and high explosive.

In this work, an experimental procedure to crystallize inorganic oxidizer salts inside the pores of nanoporous carbon is developed, the influence of the textural and surface properties of the nanoporous carbon are discussed and the obtained energetic nanomaterial is characterized in terms of structure and energetic properties.

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New ligands and energetic coordination compounds for use as primary and laser ignitable explosives

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Keywords: energetic coordination compound; primary explosive; laser ignition; tetrazole; structure elucidation.

The reliable but highly harmful compounds lead azide and lead styphnate still dominate the field of primary explosives being applied in most ignition and initiation systems to this day. Therefore, an extensive investigation into energetic materials led to the very promising strategy of developing energetic coordination compounds (ECC) with similar performance and minimized toxicity. Energetic coordination compounds can easily be tuned toward their resulting performance and sensitivities by varying the metal center, the ligand system, and the corresponding anion. In the present study, the new ligands 1-(2-azidoethyl-5H-tetrazole) and 1-(3-azidopropyl-5-tetrazole), were coordinated to different metal centers (e.g. Fe, Cu, Ag) and compared to each other. The ligands were synthesized starting from 2-chloroethyl-1-ammonium chloride and the corresponding propyl derivative. In addition, the ligands 1- and 2-amino-5-tetrazole as well as 1- and 2-amino-5-methyl-tetrazole were applied and several highly energetic complexes characterized. Furthermore, the influence of the additional methyl group on the coordination sphere and the resulting difference of the energetic properties were investigated. Characterization includes XRD, IR, EA, DTA and sensitivity (impact, friction, and ESD) measurements as well as for selected compounds classical initiation tests (nitropenta filled detonators). Laser irradiation of the received primary explosives with near-infrared light (NIR) led to a reliable and safe ignition and expands their potential for future applications.

Study on the synthesis and properties of the initiation explosives for applications in impact detonator

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Keywords: synthesis; properties; slapper detonator; initiation explosive; crystal structure.

In this paper for the first time to systematically study the amplification synthesis process and comprehensive performance of DAAF, BPTAP and ADNI in China, and measures its mechanical sensitivity, thermal stability, detonation performance and short pulse impact initiation performance according to the national army standard. Comprehensive experiment data comparison shows the ADNI compounds has very excellent sensitivity performance. The detonation velocity for ADNI (7.8 km•s-1 at a density of 1.67 g•cm-3) is greater than that of LLM-105 (7.54 km•s-1 at the density of 1.63 g•cm-3) and haxanitrostilbene (HNS) (6.8 km•s-1). ADNI also has a higher decomposition temperature (Td =265.8 °C) and a better thermal stability (5S shotpoint of 312 °C) with low impact, friction, and electric spark sensitivities (>40 N, >360 N, and 2.20 J). The uniform sub-micrometer ADNI has better sensitivity to short impulse shock waves with the 50% and 99.9% initiation currents at 2.45 kA and 2.67 kA, respectively, which is much better than sub-micrometer LLM-105 (3.11 kA and 3.46 kA, respectively) and DAAF (3.7 kA and 4.75 kA, respectively).

Kinetic and thermochemical studies of 2,4-bis(dimethylamino)-6-trinitromethyl-1,3,5-triazine

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Keywords: triazine; thermal properties; polymorphous transitions.

The thermal transformations of the high-energetic compound 2,4-bis(N,N-dimethylamino)-6-trinitromethyl-1,3,5-triazine were studied in the temperature range 170 – 623 K by means of DSC, mass spectrometry, IR spectroscopy, single-crystal and powder X-ray diffraction. The studied compound is characterized by a strong anisotropy of thermal expansion and at a temperature of about 365 K undergoes a polymorphic transformation alpha into betta, which is preceded by an abrupt drop in density. Melting of 2,4-bis(N,N-dimethylamino)-6-trinitromethyl-1,3,5-triazine (at a temperature of about 396 K) is accompanied by a sharp acceleration of thermal decomposition. The thermal effects of polymorphic transformation, melting and decomposition were measured, and the kinetics of thermal decomposition of 2,4-bis (N,N-dimethylamino)-6-trinitromethyl-1,3,5-triazine was studied. The activation parameters of the reaction in the melt and in the solution are, respectively, 102.0±4.1 and 87.9±3.2 kJ/mol; 107.31±0.6 and 107.80±0.5 s–1. The composition of the resulting gaseous products has been determined and a decomposition mechanism has been proposed, according to which the tertiary amino group is oxidized by a nitro group in the rate determining stage of the process. An anomalous kinetic behavior was found for the investigated substance: the reaction slows down sharply when passing from the melt to the solution. This fact is explained by the contribution of bimolecular reactions to the total kinetics of the process. This also explains the abnormally low values of activation parameters.

Research on performance of CL-20 based explosives with different binder systems

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Keywords: CL-20; mechanical granulating; mechanical sensitivity; compatibility.

Three types of thermoplastics elastomer A, B, C constitute the binder systems with wax respectively. Raw CL-20 was added with a small amount of graphite. The mould powder of CL-20 composite explosive was obtained by mechanical granulating technology. The experiment results showed that elastomer B was better than A and C when the mass percentage of binder systems was fixed at 5.4%. Impact sensitivity of was decreased to 16%, while the friction explosion probability was decreased to 20%. Thermogravimetric analysis (TG) revealed that elastomer B and CL-20 are well compatible. The formulation was optimized by varying the percentages of elastomer B and wax, and the mechanical sensitivity was further decreased. 20% Al powder was added into the formulation. The alumininized formulation was well coaded, thermally stable, and the mechanical sensitivity can meet the requirements of composite explosive.

Phlegmatization of energetic materials with polymer films in supercritical conditions

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Keywords: phlegmatization; HMX; CL-20; coating; particles; scco2.

A simple and effective method of coating of 1,3,5,7-tetranitro-1,3,5,7-tetrazocane (HMX) and 2,4,6,8,10,-12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) particles with fine films of polymethylacrilate (PMA), polyurethane rubbers Desmocoll-400 and Surel-9 has been developed. The coating was conducted in the supercritical carbon dioxide medium using the gas anti-solvent method (GAS). This method was previously used to cover CL-20 particles with hydroxyl-terminated polybutadiene (HTPB) but for the first time we applied it for HMX phlegmatization. In this process the supercritical fluid is used as an anti-solvent that causes precipitation of the polymer dissolved initially in a liquid solvent. Since PMA and polyurethane rubbers are components of most polymeric binders in energetic composites the use of 1-3 % wt. of them will not significantly decrease energetic parameters of the final product. Along with this, a higher flowability and significantly lower sensitivity to impact (1.7-7.8 times) and friction (1.4-1.9 times) have been obtained, compared to the original compounds. Obtained powders exhibit the increased flowability which is beneficial for manufacturing. These advantages of the coated particles correspond to the quality of their surfaces analyzed with scanning electron microscopy, as well as probe atomic force and electric force microscopy. The achieved level of phlegmatization makes it possible to increase the proportion of energetic materials in the formulation without compromising the safety of production.

Reaction of S,S'-dimethyl-N-nitroimidodithiocarbonate with 3,5-diamino-1,2,4-triazole

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Keywords: S,S'-dimethyl-N-nitroimidodithiocarbonate; 3,5-diamino-1,2,4-triazole; guanozole.

Reaction of S,S'-dimethyl-N-nitroimidodithiocarbonate with 3,5-diamino-1,2,4-triazole has been investigated. The product of the reaction of nucleophilic monosubstitution is 3,5-diamino-1-(2-methyl-1-nitroisothiocarbamyl)-1,2,4-triazole. That is, the reaction of nucleophilic substitution proceeds not through amino groups, but through the nitrogen atom in the position 1 of the 1,2,4-triazole cycle. The synthesized compound is a promising starting material for the synthesis of a number of new energetic compounds. Further reactions of compound with various nucleophilic agents were studied. The resulting compound has been studied by mass-spectrometry and elemental analysis, as well as studied by NMR, FTIR and UV spectroscopy.

On the calculated detonation parameters of some oxygen-free explosives

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Keywords: oxygen-free explosives; BKW; detonation parameters.

In recent years, a large number of articles have appeared on the synthesis of new explosives that do not contain oxygen. The heat of the explosion in them is realized not due to the oxidation of carbon and hydrogen by oxygen, as in conventional explosives like TNT or RDX, but due to the high positive enthalpy of formation of the explosive itself. For these explosives, only calculated values of detonation parameters are given, which are at the level of known powerful explosives, or even surpass them. In our opinion, these estimates are greatly overestimated. Our estimates (both using the BKW equation of state and different correlation methods) show significantly lower values of detonation parameters. The analysis of the probable causes of the overestimation of the calculated values of detonation parameters is discussed in this article.

Assessment of influence of high-intensity mechanical treatment on the properties of cellulose nitrate

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Keywords: cellulose nitrate; nanoparticles; nanocellulose nitrate; properties.

This paper presents the results of a study of the effect of high-intensity mechanical treatment on the structural and physicochemical properties of cellulose nitrates. The characteristics of cellulose nitrate were evaluated by electron microscopy, X-ray diffraction, FTIR, viscometry and elemental analysis. The results show that after high-intensity mechanical treatment occurs significant reduction in thickness of the fibers to a value of about 100 -200nm. The high-intensity mechanical treatment has no significant effect on the molecular composition of the cellulose nitrate and the average molecular weight is reduced by about 20%.

Determination of the thermal kinetiks parameters of gun propellant

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Keywords: kinetic parameters; gun propellants; thermal stability; auto-ignition.

The thermal stability of two simple base gun propellants, SB1 manufactured in 2005 and SB2 manufactured in 2011 was evaluated by determination of thermal degradation energy (Ea) using different tests such as: auto-ignition. Firstly, the stability was tested using methyl-violet and Bergmann-Junk tests. Then, the auto-ignition technique was used to determine the thermal degradation energy using isothermal and non-isothermal mode. In the isothermal mode, the value of activation energy was investigated using Arrhenius equation whereas in the non-isothermal mode, Kissenger and Ozawa were used. All the tests performed show that the thermal degradation energy of SB1 is lower than that of SB2 which exhibit the existence of a good correlation between them.

New energetic oxetane monomers based on nitroaromatic scaffolds

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Keywords: explosives; energetic monomers; energetic binders; ring-opening polymerization; oxetane chemistry.

In recent years, oxetanes have attracted lots of interest due to their ability to replace gem-dimethyl groups and to thereby enhance the polarity of medically active substances. The discovery motivated intensive research aiming at the replacement of other structural motifs by oxetanes, leading to an improved insight into the underlying chemistry and rather complex oxetane-based compounds became known to literature. This knowledge can be utilized for the synthesis of new oxetane-based monomers which may surpass state-of-the-art monomers (e.g. AMMO, BAMO, NMMO) regarding the relative complexity and energetic performance. Thus, the synthesis of novel energetic monomers based on commercially available oxetan-3-ol and easily accessible BMHMO (3-bromomethyl-3-hydroxymethyloxetane) is described. The energy content is mainly provided by classical nitroaromatic scaffolds arising from 1-halo-2,4,6-trinitrobenzenes as well as 2,4,6-trinitrobenzoyl chloride. In some cases, azido-moieties are grafted to the monomer scaffold to obtain a higher heat of formation. The resulting monomers are suitable for cationic ring-opening polymerization using a boron trifluoride etherate/diol initiator system and possess both energetic performance and thermal stability required for the application of a corresponding homo- or copolymer as energetic binder. Due to the present nitroaromatic motifs, corresponding polymers are promising candidates for an adhesion promoter-free application when applied to secondary explosives with a similar chemical structure. The compounds prepared were intensively characterized by multinuclear NMR- and IR-spectroscopy, mass spectrometry, elemental analysis, differential thermal analysis and single crystal X-ray crystallography. The sensitivity towards external stimuli like shock, friction or electrostatic discharge was determined according to BAM standard procedures.

5,5´-Dinitramino-3,3´-bi(1,2,4-oxadiazole) and its energetic salts -a series of energetic materials with good performance

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Keywords: energetic materials; 5,5´-dinitramino-3,3´-bi(1,2,4-oxadiazole); energetic saltsd.

In this work, 5,5´-dinitramino-3,3´-bi(1,2,4-oxadiazole) (3, DNABO), a new heterocyclic energetic compound, was synthesized by the simple nitration of 5,5´-diamino-3,3´-bi(1,2,4-oxadiazole) (2) with 95% fuming nitric acid. By treating compound 3 with two equivalents of energetic bases or their salts, a serial of energetic salts 4-10 based on nitrogen-rich cations were readily obtained. Among them, the hydroxylammonium salt (5) shows the best comprehensive properties (5: d=1.879 g cm-3; Td=190 oC; P=36.2 GPa; vD=8916 m s-1). Additionally, the guanidinium salt (7) possesses excellent thermal stability with an onset decomposition temperature of 317oC.

Determination of combustion temperature of energetic materials based on nitrates of various metals at atmospheric pressure

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Keywords: combustion temperature; energetic materials; potassium nitrate; sodium nitrate; tungsten-rhenium thermocouples.

The experimental and theoretical combustion temperature of the systems based on plasticized phenol-formaldehyde resin and nitrates of various metals at atmospheric pressure was determined. For the samples based on alkali and alkaline metal nitrates, they are somewhat different from the theoretical temperature at atmospheric pressure.

Strategy for the design of new ionic liquids to replace hydrazines in rocket propulsion

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Keywords: rocket propulsion; ionic liquid; chemical synthesis; performance; desensitization; differential scanning calorimetry.

This paper describes our work on the design of new (room temperature) ionic liquids initiated by remote control, thus, avoiding the catalytic decomposition of the propellant. The design of such systems should allow attaining higher levels of performance in comparison to hydrazine-based propellants and the development of REACH-compliant alternatives.

Investigation of the molecular and crystal structure of two 2,4,6-trinitrobenzene derivatives

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Keywords: 2,4,6-trinitrobenzaldehyde; 1-fluoro-2,4,6-trinitrobenzene; crystal structure; 2,4,6-trinitrobenzene.

The molecular and crystal structure of two derivatives of 2,4,6-trinitrobenzene was determined. For 2,4,6-trinitrobenzaldehyde (1): orthorhombic, Pbcn, a = 10.5782(10), b = 14.2749(16), c = 12.0267(13) Å, α = 90°, β = 90°, γ = 90°, V = 1816.1(3) Å3, Z = 8, D = 1.764 g cm-1, wR2 = 0.0955, R1 = 0.0437; GooF = 1.042. For 1-fluoro-2,4,6-trinitrobenzene (2): orthorhombic, Pca21, a = 9.1070(7), b = 18.737(2), c = 9.7887(8) Å, α = 90°, β = 90°, γ = 90°, V = 1670.3(3) Å3, Z = 8, D = 1.838 g cm-1; wR2 = 0.1427, R1 = 0.0637, GooF = 1.012. The fluoro derivative (2) crystallizes with two crystallographically independent molecules in the asymmetric unit. The new structures of the two derivatives of 2,4,6-trinitrobenzene are compared to the literature known structures of 1-trifluoromethyl-2,4,6-trinitrobenzene (3), 2,4,6-trinitrobenzamide (4) and 2,4,6-trinitrobenzoic acid (5). The presence of the aldehyde function in (1) causes a significant twist of one of the neighboring nitro groups, which is discussed in terms of the steric situation in the molecule as well as in terms of H-bonding. In contrast, the fluorine substituent at 1-position in (2) only induces a very light twisting of the neighboring nitro groups when compared to (1) and the literature known compounds (3) - (5). The influence of the substituent in 1-position on the angles, distances and torsion angles within the molecule as well as its impact on the intermolecular interactions between the individual molecules in the unit cell are described and discussed. This interplay, supported by the rotational flexibility of the nitro substituents, results in a very interesting three-dimensional arrangement of the molecules in the crystal structures of (1) and (2).

Investigating the plateau burning of composite solid rocket propellants based on different isocyanates

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Keywords: plateau burning; composite propellant; hydroxyl-terminated polybutadiene (HTPB); ammonium perchlorate; Crawford bomb.

Plateau burning of composite solid rocket propellants is a required goal in the design of propulsion systems for space launching vehicles and military missiles. In this study, we aimed to generate plateau burning from abundant and processing-friendly curing agents. Therefore, three propellant compositions were prepared based on changing the employed isocyanate namely, hexa-methylene di-isocyanate (HMDI), iso-phorone di-isocyanate (IPDI) and di-cyclohyxyl-methane di-isocyanate (H12MDI) to investigate their ability to generate plateau burning. The burning rate of these compositions was measured at 1 MPa-intervals from 1-14 MPa via Crawford bomb to study its response to different pressure regions. While compositions based on HMDI and IPDI exhibited bi-plateau and plateau burning phenomena respectively, the H12MDI composition did not show any abnormal behavior at the examined pressure range. These results is related to the activation energy of the first decomposition stage of the employed binders, which is believed to be responsible for the existence of the plateau burning. The higher the decomposition activation energy of the binder was found to absorb more energy from the surrounding burning surface, thus causing less thermal energy to be delivered to the coarse ammonium perchlorate to burn. This would cause a slight depression in the structure of the flame of coarse ammonium perchlorate consequently causing the plateau burning to exist.

Octyl-1-azide as modifier of HTPB

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Keywords: HTPB; chemical modification; azide molecule; propellant; binder.

Hydroxyl terminated polybutadiene (HTPB) has been several times modified and copolymerized with azide substances to be applicable as an elastomer binder in a composite solid propellant (CSP). This research presents the chemical modification of the HTPB with octyl-1-azide (OAz) carried out through the bulk reaction between the HTPB double bonds and azide pendant groups. The formation of carbon-nitrogen bonds were evaluated by Fourier transform infrared spectroscopy (FTIR) and 1H Nuclear Magnetic Resonance (1H NMR). Through size exclusion chromatography (SEC), the slight molar mass increase was calculated. The final product was also characterized by differential scanning calorimetry (DSC) and by oscillatory disc rheometer, which revealed, respectively, a glass transition temperature (Tg) and viscosity values which are in the range for elastomers to be applied as binders in CSP.

The model of polychromatic kinetics of solid-phase reactions and its application for the analysis of the kinetics of thermal decomposition of fuel for a gas generator of a ramjet engine

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Keywords: polychromatic kinetics; dispersion of reactivity; thermal decomposition of solid fuel; ramjet; integral equation of the first type; inverse problem.

The kinetics of chemical transformations of solid-fuel compositions is distinguished by the following fundamental feature of solid-phase reactions: in the isothermal mode, the reaction, when it reaches a certain degree of conversion, depending on temperature, can practically stop. However, with a subsequent increase in temperature, the process rate increase again. This effect cannot be described by single component kinetics. The reasons for such phenomena have long been debated, but have not yet received an established theoretical explanation. The solution of such kinetic problems is necessary, for example, to analyze the stability of aircraft fuels. Solid fuels of high-speed aircraft can be exposed to both high and low temperatures, which, in turn, can lead to changes in the composition due to reactions occurring during thermal decomposition, and in the case of insufficient heat removal - and ignition. Therefore, it is very important to know the kinetic characteristics of the thermal decomposition of fuel compositions. In this paper, we use the concept of the presence in the condensed system of a family of particles ensembles with a reactivity dispersion, which is mathematically formalized as a so-called polychromatic kinetic model. This model connects the observable kinetic characteristics with the distribution function of the parameters of the reactions of particles in the ensemble by means of a first kind integral equation. As an example of the application of the model, the kinetics of mass reduction during heating of standard solid fuel to temperatures of 300°C in closed and open systems is investigated. It is shown that the kinetic curves of mass reduction in air atmosphere have a pronounced stepped character under isothermal conditions. The formulation and numerical solution of the corresponding inverse problem was carried out, which made it possible to explain the set of kinetic data describing the mass reduction as a result of linear heating at different rates.

Physico-chemical properties of nitrocellulose granular with different nitrogen content

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Keywords: nitrocellulose; nitrogen content; spherical powder.

Nitrocellulose (NC) is a high-energetic polymer with good physico-chemical properties and it can be processed to different shapes (flakes, cylinders, spherical balls). NC granules are used for solid rocket propellants (homogeneous propellants) or gun ammunition (spherical powders). NC granules were obtained by water method in laboratory scale – it's safe method for the production of spherical powder, because NC was suspended in water. The used NC was characterized by different viscosity and nitrogen content in the range of 12,3-13,3%. Other process components were: ethyl acetate as solvent, centralite I as stabilizer, starch as protective colloid, sodium sulfate as dehydrating agent. Physico-chemical properties of obtained granules were examined, e.g. thermal properties, density, heat of combustion. The influence of nitrogen content on the properties of obtained NC granules was determined in this work.

Calculated molecular properties and possible performance of several azidotetrazoles

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Keywords: azidotetrazole; molecular property; performance; decomposition mechanism; detonation wave.

A lot of new calculated results were obtained for six azidotetrazoles such as 5-azidotetrazole, 1-amino-5-azidotetrazole, 1-(aminopropan-2-ylidene)-5-azidotetrazole, 1-(aminoazidocarbamoyl)-5-azidotetrazole, 5-azido-1-diazidocarbamoyltetrazole and 1,2-bis(5-azidotetrazol-1-yl)ethane. Quantum chemistry methods implemented in the Gaussian 09 computer program were used first of all. The method of density functional theory with the B3LYP hybrid functional was used for a number of basis sets, from 3-21G to 6-311+G(2d,2p). The overwhelming number of calculations were carried out with the spin-polarized 6-31+G(d) basis set. Some comparative calculations were also carried out using complete basis set (CBS-4M, CBS-QB3, CBS-APNO) and Gaussian-n (G3, G4) more precise methods. All major geometric and energetic properties of explosive molecules were determined. The main attention was concentrated on the investigation of primary decomposition mechanisms of the molecules considered. It was obtained that these mechanisms were primarily characterized by the destruction of the azide groups and tetrazole rings. The energy barriers and energy effects of these reactions were determined and compared for all molecules. The enthalpies of formation of all explosive substances in the gas phase were determined using the specified precise calculation methods. The enthalpies of sublimation required for obtaining the enthalpies of formation in the solid phase were determined using several empirical methods. The confidence intervals of the obtained sublimation enthalpy values were estimated on the basis of orientation accuracy of the empirical methods used. These data were then used for estimating the possible performance of explosives considered. All characteristics of detonation waves and detonation products were calculated using the EXPLO5 thermochemical program. The parameters of the equations of state for detonation products in the form of Jones-Wilkins-Lee were determined too. A number of calculations of exploding action of explosives were conducted using the ANSYS Autodyn gasdynamic program. The explosions of thin layers of pure and polymer-bonded explosives on thick barriers in normal and bulk detonation modes were considered.

Solving the problems of detonation and combustion of different energetic materials using the Explo5 program

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Keywords: thermochemical program; energetic materials; detonation; combustion; equations of state.

A lot of new calculated results on thermochemistry, thermodynamics and performance of energetic materials using the V6.04 latest version of the thermochemical Explo5 program are presented in the work. A wide range of energetic materials such as high explosives, gunpowders and solid rocket propellants were considered. In the first introductory part of the work, a brief description of the structure and capabilities of the program used and the calculation methods involved are given. The large and repeatedly tested database of parameters for reagents, reaction products and used equations of state is presented and the methods of its extension are indicated. In the second also rather brief part, the results of combustion calculations for a number of propellants in the adiabatic approximation are presented for the constant pressure and constant volume conditions. In the third main part of the work, the numerous results of detonation calculations for RDX, HMX and TATB formulations are presented. Two models are used for detonation calculations: the Zeldovich-Neumann-Döring ideal detonation model and the simple Wood-Kirkwood non-ideal detonation model. As a result of performed calculations, all flow parameters of the considered processes were obtained, the compositions and thermodynamic characteristics of the products of detonation as well as of combustion at all their stages were determined. In the case of detonation, all parameters of detonation waves such as detonation velocity, detonation pressure, the heat detonation and so on were determined too. Based on the obtained results of isentropic expansion of detonation products, the parameters of their equations of state in the form of Jones-Wilkins-Lee were calculated for all explosives in various initial states. In the case of using the non-ideal detonation model, all such results were obtained for a concrete diameter of the charge and the reaction zone lengths were calculated too. All the results thus obtained were compared with known experimental data and with calculations performed using other thermochemical programs.

Impact sensitivities of explosives explored by the OZM ball drop tester (BIT-132)

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Keywords: ball drop; sensitivity; impact energy; explosive.

Safety, performance and toxicity are the most important aspects of modern explosives. Sensitivity measurements are carried out in different manners all around the world, often making a comparison of the results difficult. Due to this, we present our first results on the novel ball drop tester (BIT-132), manufactured by OZM research, following MIL-STD-1751A (method 1016). The sensitivity tester is a device, dropping a free-falling steel ball onto an unconfined sample, assumed to produce results more realistic than currently used methods like the BAM drophammer. Common primary explosives (lead azide, lead styphnate, silver azide, KDNBF, K2DNABT, tetrazene and others) as well as secondary explosives (PETN, RDX, TKX-50 and others) were chosen for evaluation. The results according to the probit-method were compared to the energies observed by the BAM drophammer. The differences between the results of both methods as well as ad- and disadvantages are discussed.

Synthesis of a new energetic metal-organic framework based on Gem-dinitromethyl substituted 1,2,3-triazole

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Keywords: metal-organic framework; 1,2,3-triazole; high energy; green energetic material.

In this work, through controllable synthesis, energetic metal-organic framework gem-dinitromethyl substituted dipotassium 4,5-bis(dinitromethyl)-1,2,3-triazole with "cage-like" crystal packing was obtained and characterized. Most importantly, for the first time we found that it could be successfully afforded with the catalytic effect of trifluoroacetic acid. Dipotassium 4,5-bis(dinitromethyl)-1,2,3-triazole was fully characterized by IR spectroscopy ,elemental analysis, NMR spectroscopy (^{1}H and ^{13}C) and differential scaning cabrimetry(DSC). This new compound exhibited its high density (2.04 g/cm^{3}) at ambient temperature, superior detonation velocity (8715 m/s) to that of lead azide (5877 m/s) and comparable to that of RDX (8748 m/s). Its detonation products are mainly N_2 (48.1 %), suggesting it is also a green energetic material. The above-mentioned performance indicates its potential applications in detonator devices as lead-free primary explosive.

Manufacture and study of Composition C-4 formulated by the organic solvent-free water slurry coating (OF-WSC) method

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Keywords: Composition C-4; Organic Solvent-Free Water Slurry coating.

We formulated the Composition C-4 by the organic solvent-free water slurry coating (OF-WSC) method using polyisobutylene emulsion and sequantial extrusion process of produced molding powders made the final blocks with desired shape and size. Their performance parameters including detonation velocity, detonation pressure, critical diameter, and sensitivity to impact, friction and shock were measured. The malleability of produced C-4 also demonstrated on the curved or rounded objects in the study.

Mixtures of pentaammine (5-nitrotetrazolato – N2) cobalt (III) perchlorate and nanocarbon

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Keywords: energetic complex; allotropic forms of nanocarbon.

It is known to use allotropic forms of nanocarbon (NC) (fullerenes (C60) - 0D, nanotubes -1D, graphene - 2D, detonation nanodiamonds (DND) - 3D) for modifying of the performance properties of energetic materials (EM). The purpose of this work was to determine the effect of NC additives on the properties of the energetic complex — pentaammine (5-nitrotetrazolato – N2) cobalt (III) perchlorate (NCP). The 0D and 3D nanocarbons used in the work were from Sigma Aldrich (USA). 2D carbon structures were obtained according to the original technology of carbonization of biopolymers developed by us under the conditions of the process of self-propagating high-temperature synthesis. The obtained material in its morphometric parameters corresponded to multilayer graphene - GnP. Mixtures of NCP and NC were obtained by sonication by ultrasound (US) (60 minutes) of the corresponding suspensions in the medium of an organic solvent. The obtained powders were studied by the methods of electron microscopy and Fourier IR spectroscopy. Our experiments showed that the obtained powders are a composition of NCP (with an average crystal size of 10–20 μm) and NC particles (with minimum size of 20 nm). IR spectroscopy showed that the mixture of NCP and C60 did not have any specific features and showed superposition of the complex and fullerene spectra, which indicates the absence of specific interactions between the components of the mixture. Analysis of the IR spectrum of NCP and DND mixture showed the interaction between the surfaces of NCP and DND, leading to a change in the surface structure of DND particles. IR spectra of the mixture of NCP and GnP showed the presence of interaction of the mixture components. Moreover, both ammonia and nitrotetrazole ligand are involved in the interaction. The temperatures of the onset of decomposition (Tod.) and the temperature of the onset of the intensive decomposition (Toid.) of samples NCP and its mixtures with NC were inves

Blast effect and thermal measurements of thermobaric explosions in open terrain and enclosures

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Keywords: thermobaric; overpressure; numerical simulation; postcombustion.

The experience of the latest military conflicts has shown the urban area as a space for combat. New types of asymmetric conflicts as well as global urbanization will require the transformation of combat tactics and, implicitly, weaponry used to wage fighting in urban areas. The urban area is dominated by buildings and structures with solid reinforced concrete structure. These spaces are real shelters for the insurgent elements present in the battlefield. To help eliminate the risks and threats specific to the enemy in urban guerrilla formations it is necessary to equip combat units with weapon systems capable of neutralizing the enemy forces housed in buildings, buried shelters, bunkers, tunnels or leading to the destruction of these structures. Thermobaric weapons are part of the airdispersed explosive systems family, known as "volumetric weapons". This family includes both fuel-air-explosive (FAE) and thermobaric explosive systems. The term used for naming this class of explosives originates from the Greek words "therme" and "baros", meaning "temperature" and "pressure", referring to the main destruction mechanisms for the operation of this type of weaponry. The destructive characteristics of these types of weapons are based on incendiary ability and shock wave. Both thermobaric and FAE systems are based on the same functional principle. In order to asses the destructive effects of thermobaric weapons, pressure measurements and thermal high speed video is used in order to compare the effects with TNT. For the pressure measurements, the open air configuration is complemented by measurements in semi confined spaces and closed spaces.

Early events when heating 5,5'-bis(2,4,6-trinitrophenyl)-2,2-bi(1,3,4-oxadiazole): Self-consistent charge densityfunctional tight-binding molecular dynamics simulations

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Keywords: thermal decomposition; molecular dynamics; DFT calculations.

The thermal decomposition of heat resistance explosive 5,5'-bis(2,4,6-trinitrophenyl)-2,2-bi(1,3,4-oxadiazole), also known as TKX-55, is investigated by self-consistent charge density-functional tight-binding method combined with molecular dynamics (MD) simulations. Constant temperature heating and temperature-programmed heating are employed to study the decomposition process. Three different initial decomposition reactions, involving C-NO2 bond cleavage and ring opening through the breaking of C-N bond, are found in the temperature-programmed heating simulation from 300 to 3000 K, while only ring opening is found in the constant temperature heating simulation at 3000 K. The reactants and products development as a function of temperature is supplied. Static DFT calculations show that the ring opening reactions are the most energetically favored. These findings are expected to deepen the insight into the thermal decay mechanism of energetic materials.

Studying gasification of paraffin based fuels upon blowing by moderate temperature air flow

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Keywords: paraffin; entrainment; gasification; blowing; microwave.

At present the interest in hybrid and ramjet rockets becomes actual that, in turn, leads to searching the high-energy systems / components corresponding to these tasks. Typical components of rocket propellants in the conditions of high-speed gas blowing demonstrate the poor speed of gasification. One of the directions of searching promising fuels consists in use of paraffin based compositions. Paraffin is high-energy hydrocarbon with low melting point. Along with the low viscosity this provides substantially enhanced gasification rate in the conditions of high-speed blowing. Besides, it is expected that the liquid fuel enable an additional mass transfer by entrainment of liquid droplets. Results of studying the behavior of mixes of paraffin with various additives in the conditions of intensive blowing at pressure of 10 atm by hot air with temperature 470 K are given in this work. As 10% by mass additives the stearic acid, Alex nanoaluminum, aluminum hydride, boron and mechanoactivated AlB2 were used. Experiments were conducted using the samples of cylindrical form with the central channel. By means of the microwave gage of original design the diameter of a channel was measured during the experiment in real time with subsequent calculation of gasification rate. Also the measurements of a temperature profile in the condensed phase were taken. By results of this research the physical model of gasification of paraffin fuel when blowing by hot air has been formulated.

The thermochemical properties of nitrourea and its salts

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Keywords: nitrourea; calorimetric method; enthalpy of formation; enthalpy of dissolution.

Enthalpies of formation and dissolution of nitrourea and its hydrazinium salts are measured thanks to complex use of precision calorimetric methods of burning and dissolution. As a result the enthalpy of formation of an anion of nitrourea is received from two groups of independent data and has made -59,3 +- 0,1 kcal·mol-1. Enthalpies of formation of sodium and potassium salts of nitrourea in a standard condition are defined on the basis measured their enthalpies of dissolution and received value the enthalpy of formation of an anion of nitrourea. The got value of an enthalpy of formation of an anion of nitrourea allows to measure by a method of dissolution of an enthalpy of formation of metal any salts of nitrourea.

The boron-containing components in high energy materials

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Keywords: high energy; boron; aluminum diboride; ignition; activation energy.

The paper presents the measurement results of ignition and thermal decomposition process of high-energy materials (HEMs) samples based on perchlorate and ammonium nitrate, active binder and powders of Al, B, AlB2, and AlB12. We investigated HEM ignition process with the use of set up for the radiant heating on the basis CO2-laser in the heat flux density range of q = 90–200 W/cm2. We determined the activation energy and ignition characteristics for the HEM samples with metal powders. It was found that the complete replacement of aluminum micro-sized powder by amorphous boron in the HEM composition leads to a considerable decrease in the ignition delay time for the sample by 2.2–2.8 times for the same values of heat flux density due to high chemical activity and the difference in the oxidation mechanism of boron particles. The use of aluminum diboride in the HEM composition allows to reduce the ignition delay time of HEM comparison by 1.7–2.2 times.

Thermal decomposition of some cyclic N-nitrosamines under non-isothermal conditions

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Keywords: thermal decomposition; cyclic N-nitrosamines; characteristic temperatures; activation parameters.

The thermal decomposition of 1,3,5-trinitrozo-1,3,5-triazacyclohexane (TMTA) and 3,7-dinitrozo-1,3,5,7-tetraazabicyclo[3.3.1]nonane (DNPT) is investigated by the method of derivatography using chromato-mass spectrometry. The characteristic temperatures and activation parameters of thermal decomposition are determined. The mechanism of thermal decomposition is established.

Thermal decomposition of 1-R-gem-dinitropropyl substituted 4,4,6,6-tetranitro-2,8-dioxacyclooctane

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Keywords: thermal decomposition; gem-dinitro compounds; kinetic parameters; reactivity.

Thermal decomposition of 1-R-gem-dinitropropylsubstituted compounds on the base of 4,4,6,6-tetranitro-2,8-dioxacyclooctane in solution of dibutyl phthalate proceeds by the homolytic mechanism with break of C-NO2 bond in one of gem-dinitromethyl groups in dioxacyclooctane. For the limiting stage the kinetic parameters are determined. In dinitropropyl fragment of molecule the steric effect of α-substituent significantly influences on the thermal decomposition rate of germinal dinitro group. Increase of substituent volume leads to increase in the magnitude of the rate constant of reaction. The quantitative relationships between the logarithm of the rate constants, activation energy and steric constants of substituents are found, from which it is possible to construct the molecules with preset parameters on chemical stability.

Green is the new black: an environmentally benign black smoke fulfilling the concept of fuel mixes

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Keywords: pyrotechnics; smokes; black; fuel mixes.

The concept of fuel mixes, which was established to generate multi-colored smoke signals with the colors red, violet, yellow and green, was extended by an additional black color impression. The underlying pyrotechnical system is based on commercially available potassium chlorate, 5-amino-1H-tetrazole and a magnesium carbonate derivative. In contrast to further naphthalene-based smoke mixtures, the black color was produced by mixing a green and red smoke dye (Solvent Green 3/Disperse Red 9) as a much greener alternative. By using the same dyes as for red and green smoke, it was possible to apply a consistent pyrotechnical system with known performance. Standard methods of characterizing smokes according to their burning behavior, yield and energetic properties were used to estimate the effectiveness. Further, the new black-smoking compositions were compared to the already existing multi-colored smoke formulations.

Planarity of shock wave from explosive plane wave generator

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Keywords: plain wave generator; PWG; planar shock; explosives.

In a case of our small-scale experiments we are often facing the trouble with not planar shock wave front generated by a detonation of high explosive. For many applications in detonics and shock wave physics the shock front planarity is a necessary precondition. Thus, we have been developing a cheap, available plane wave generator.

In this paper we are briefly summarizing our results from several approaches tested to shape the detonation front. We began with measurement of detonation front curvature of bare A IX-1 charge in few different L/D ratios. Then, a simple inert PMMA insert and accelerated aluminium liner were used. Most recently, we tried approach using inert metal ring inserted between two A IX-1 charges to create a planar shock front. The planarity was evaluated by ultra-high-speed imaging, passive optical system OPTIMEX and laser interferometry (PDV).

Conclusions of the thermal stability Round-Robin tests among Notified Bodies

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Keywords: 75°C/48h; proficiency test.

The ISO/IEC 17025:2005 standard establishes that the laboratory shall have quality control procedures for monitoring the validity of their tests. For this monitoring participation in proficiency testing may be used. It was agreed amongst the Notified Bodies for Explosives, that the upcoming proficiency testing would concern the thermal stability testing (75°C/48h) in accordance with the EN 13631-2:2003 standard. As there were no special chemicals found to fail to the test, special compositions have to be developed. This paper describes the development, the evaluation and the conclusions of the Round Robin test, which pointed out the necessity of the recast of the EN 13631-2 standard.

Simultaneous measurement of detonation velocity & detonation front curvature using fiber optic probe

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Keywords: fiber optic probe; detonation wave curvature; detonation velocity; erythritol tetranitrate.

The paper describes a novel technique of measurement of two key parameters of detonation wave, velocity and front curvature, at the same section of a cylindrical explosive charge. The measurement technique utilizes a perforated fiber optic probe which crosses the tested charge under an angle of 45°. Small holes drilled in the probe core act as air voids and produce light pulses upon arrival of the detonation wave. The curved front of the detonation wave passing along this probe causes nonlinear time distribution of the light pulses which can be analyzed to determine both detonation velocity and shock front curvature. The technique was tested on melt casted charges of erythritol tetranitrate and also on a powdered mixture of ammonium nitrate and aluminium. The resulting detonation velocity was in a perfect agreement with previously measured and calculated values.

Effect of suspension composition on electrophoretic deposition and combustion properties of Al-CuOx nanothermite material for on-chip energetics

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Keywords: powder nanothermites; electrophoretic deposition; combustion; MICs; initiators.

Today the active development of MEMS, systems on a chip and other miniature devices has become an engine for the development of various types of integrated energy sources. Local heat sources can be used for packaging and bonding, to initiate secondary reactions, or to power the device. Thermite materials, which are usually made in the form of multilayer film structures, are actively used for this purpose. In this paper, the features of electrophoretic deposition of al-CuOx composite thermite materials based on powders with particle size less than 100 nm were investigated. The dependences of the sediment composition on the suspension composition were plotted, the influence of the main modes of the deposition process on the deposition rate and character was determined. The thermal effects in the formed material were measured using DSC and TGA analysis and its combustion rate were studied with high-speed videocamera. The simplicity of this method, the possibility of local deposition and control of the composition and deposition rate of the material - all this distinguishes electrophoretic deposition and opens up opportunities for its application.

Ethoxy-2,4,6-trinitrobenzene(ETNB), a new candidate for melt-cast explosives

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Keywords: ethoxy-2,4,6-trinitrobenzen; ETNB; melt-cast explosive; synthesis; detonation velocity; shock sensitivity.

ETNB has been proposed as a suitable alternative to TNT in low sensitive melt-cast formulations. Characterization of synthesized ETNB were carried out by NMR, DSC, and sensitivity and detonation property analysis. The melting point of ETNB(78 80'C)is almost the same as that of TNT(78 81'C). ETNB was found to have shock sensitivity of 52kbar and detonation velocity of 6.4km/s. Sensitivity and detonation property of ETNB based melt-cast explosive formulations will be discussed.

New 2,2,2-trinitroehylamino- and 2,2,2-trinitroethylnitramino-derivatives of azidotriazines. Synthesis, thermochemical properties and energetic potential

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Keywords: triazine; azido-derivatives; nitro-derivatives; trinitroethyl-derivatives; synthesis; enthalpy of formation; propellant; specific impulse.

New 4,6-diazido-N-(2,2,2-trinitroethyl)-1,3,5-triazine-2-amine (I); 6-azido-N2,N4-bis(2,2,2- trinitroethyl)-1,3,5-triazine-2,4-diamine (II); 6-azido-N2,N4-dinitro-N2,N4-bis(2,2,2-trinitroethyl)-1,3,5-triazine-2,4-diamine (III) and N2,N4,N6-trinitro-N2,N4,N6-tris(2,2,2-trinitroethyl)-1,3,5-triazine-2,4,6-triamine (IV) have been synthesized. Their enthalpies of formation have been determinated experimentally: 690.1±5.9; 326.2±13.6; 630.1±13.8 and 415.9±9.3 kJ/mol. Thermodynamic analysis shows that basing on compounds III and IV it is possible to create propellants with low aluminum content, achieving specific impulse value up to 257-260 s at Pc and Pa equal to 4.0 and 0.1 MPa respectively.

Potential capability of some ethynyl derivatives as fuel dispersants for solid fuel ducted rockets

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Keywords: diethinylbenzene; dispersant; fuels for direct-flow rocket engines.

The latest achievement in the chemistry of components for fuels intended for use in direct-flow rocket engines (DFRE) is the proposal to use the 1,4-diethinylbenzene (DEB) as a dispersant, which differs from many other potential dispersants not only by a high calorific value (42 MJ / kg), but also by a high combustion temperature (1980 K at 50 atm) with no external oxidizer participation. It was shown recently in the Institute of Problems of Chem.Physics, Rus.Acad.Sci. This achievement is the result of the combination of high enthalpy of formation of DEB with the absence of nitrogen and oxygen in its formulation - the presence of these elements reduces the heat of combustion of even very high-enthalpy compounds. The potentialities of some analogs of the DEB, which have not yet been synthesized, have been investigated. The values of their enthalpies of formation were evaluated and the achieved values of combustion heats and adiabatic temperatures (Tad)were compared. It was shown that components based on other aromatic frameworks (naphthalene, anthracene) lose very little to DEB in the combustion heat release , but significantly gain in terms of Tad, while components based on similar saturated structures (such as hexacyclopropane) lose essentially on Tad, although they gain a little in terms of heat of combustion

Electron beam, as a means of direct initiation of energetic materials

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Keywords: electron beam; explosives; detonation; PETN; RDX; DADNE.

The possibilities of direct initiation of pure explosives under the action of a high-density pulsed electron beam are presented. The comparative analysis of threshold characteristics of initiation for a series of explosives is carried out (PETN 14,5 J/cm^2 [1], RDX 15 J/cm^2 [2], DADNE 19.5 J/cm^2). The results show that the initiation threshold has no direct connection with the mechanical and thermal initiation thresholds. This can be explained by the fact that when the absorption of electrons in the material occurs ionization of molecules, which facilitates the launch of the explosive decomposition reaction. Due to the short impact times and good synchronization it is possible to study the stages of decomposition in real time [3].

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Fragment velocity formula for reverse detonation driving in opposite initiation

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Keywords: detonation driving; fragment velocity; one dimensional gas dynamics; multi-point initiation.

In the problems of detonation driving, the explosive charge is usually initiated in one side and drives the fragment or plate located in the other side. This driving style has lots of studies and practical applications, but less studies is done in the reverse detonation driving, where the initiation point is located at the same side of the fragment. The reverse detonation driving can lower the shock pressure in the fragment and solve the problem of spallation. The model of opposite initiation of cylindrical charge is used to study the reverse detonation driving in this work. A long element is taken along the direction of initiation points and the warhead center, and a fragment velocity formula is established according to the one dimensional gas dynamics. Then, considering the influences of assumptions like rigid constraint of the element, three experimentally verified numerical modeling are used to validate the established formula. The ratios of the formula computations and the corresponding modeling results have the almost same trends. Therefore, the similar trend are fitted together and used as correction factor of the established formula. The established formula can be used as a good reference for the problem of reverse detonation driving.

Preparation and characterization of energetic nitrotetrazolate-1N-oxides

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Keywords: tetrazole; N-oxide; explosive; sensitivity; energetic parameter.

The ongoing demand for high performing energetic materials led to the introduction of N-oxides to nitrogen-rich heterocycles. This concept has already proven its value, usually by providing an increase in density, oxygen balance and performance while offering lower sensitivities. The highly energetic 5-nitrotetrazole-1N-oxide anion (N+O = 90.76%) was made accessible for the first time, using a convenient and novel synthetic pathway. The ammonium and potassium salts were exemplarily prepared and extensively characterized using XRD, IR, EA, NMR, DTA, and sensitivity (impact, friction and electrostatic discharge) measurements. The energetic performance of the compounds was calculated using the EXPLO5 code in its latest version. The computed parameters are very promising, outperforming those observed for the isomeric 5-nitrotetrazole-2N-oxide salts.

Inclusion complexes of cyclodextrin nitrates with compounds containing explosive groups in their composition

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Keywords: inclusion complexes; cyclodextrin nitrates.

Cyclodextrins (CD) are cyclic glucose oligomers with 6, 7, and 8 glucopyranose units (α-, β- and γ-CD, respectively). An interesting and practically significant property of CD is their ability to form inclusion complexes (IC) with organic and inorganic compounds “host-guest”. In the formation of IC molecules "guest" are placed in the cavity of the CD, the molecule of which has the shape of a torus. The properties of such a complex may differ significantly from its constituent compounds. The study of these complexes is of scientific interest, they themselves can be used for practical application in various fields. The nitrates of CD (NCD) are amorphous substances and are likely to have the same toroidal structure as the original CD molecules. The ONO2 groups formed during nitration, like the initial OH groups of the CD, appear to be on the outer surface of the torus, and therefore the size of the internal cavity should not change significantly. Due to this, NCD retain the potential ability to form IC. A necessary condition for the interaction of the NCD and the substance embedded in its structure, which would lead to the formation of a complex, is not the excess of the geometric dimensions of the “guest” molecules embedded over the dimensions of the internal cavity in the NCD. An important role in the formation of IC will have not only the size of the “guest” molecule, but also its asymmetry, as well as the level of thermodynamic affinity of the components. In this work, the possibility of obtaining α-, β- and γ-NCD complexes with such compounds as isosorbid mononitrate (ISN) and nicorandil (NK) was investigated. As the initial NCD, both completely substituted α-, β- and γ-NCD, and NCD with a degree of substitution of hydroxyl groups for nitrate 55% and 83% were used. Investigated IC NCD with ISN and NK with different molar ratios of components (1: 1, 1: 2, 1: 3). The proof of the formation of complexes was carried out using X-ray phase analysis, TGA, DSC and NMR. Work was supported by the Russian Foundation for Basic Research (grant 16-29-01041 ofi-m).

Cyclic and frame hydrocarbons - the energy of reorganization of the radicals

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Keywords: enthalpy of formation; energies of the bond; radical rearrangement; adamantane; cuban.

On the basis of enthalpy of formation of cyclic and frame compounds and their radicals in the gas phase, the energies of radical rearrangement are determined. For calculations used the thermochemical data for monocyclic compounds from cyclopropane to cyclododecane and adamantane, Cuban and other substances and related radicals. In the calculations used patterns previously identified for medium thermochemical energies of the bonds of aliphatic compounds and energies of the rearrangement of the radicals.

Copolymerization of nitratomethyl and azidomethyl substituted oxetanes: the morphology of statistical block copolymers

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Keywords: 3,3-bis(azidomethyl)oxetane; 3- nitratomethyl -3-methyloxetane; block copolymers; cationic ring opening polymerisation (CROP); morphology; X-ray wide angle scattering.

The article presents research of the amorphous-crystalline and molecular structure of 3,3-bis(azidomethyl)oxetane (BAMO) and 3-nitratomethyl - 3-methyloxetane (NIMMO) copolymers with wide angle x-ray scattering and FTIR. Copolymers were synthesized by polymerization via a cationic ring-opening reaction mechanism with different amount of monomer units BAMO and NIMMO. Introducing asymmetric units presented by nitratomethyl- instead azidomethyl-groups into the structure of block copolymers allows arriving at better physical and mechanical characteristics and oxygen balance.

TNT detection with TF-BAR sensors coated with biochemical layers

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Keywords: MEMS; TF-BAR; detection; TNT; antibody.

This paper presents the development of a thin-film bulk acoustic resonator (TFBAR) sensor based system capable of multiple explosives detection. The effect on which the detection is based is represented the immobilization of explosive vapors on a layer of antibodies, and it's subsequent detection via an electro-mechanical system (MEMS). The sensor consists of a thin piezoelectric layer (ZnO, AlN or PZT below 1μm),creating a resonator working in longitudinal vibration mode, in which the resonance frequency is determined by the reverse of the piezoelectric layer thickness and directly proportional to the material constant. The reduced dimensions allow it to operate at high frequencies (1-10GHz), and with a high quality factor. A silicone wafer coated with a SiN membrane will provide the necessary support structure, and the deposition of the antibodies is achieved with the help of two intermediate layers of gold and protein, thus creating a polarized link, leaving free the antigen binding. The binding of the explosive molecules to the antibodies changes the resonance frequency of the sensor, thus detecting it's presence. The system comprises of several sensors, each of which designed with it's own type of antibodies, for specific explosives. Each biochemical layer is chosen as to provide high affinity and discriminatory capabilities. A heater ensures the vaporization and the optimum condition for the explosive-antibody binding, and a flow controller routes the vapors through a cavity beneath the sensor. A network analyser, a PC and an interface are also required. The aim is to provide a cheap, portable and user friendly system.

Synthesis and properties of new derivatives of nitroimidazole

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Keywords: imidazole; nitroimidazole; energetic substanses.

The article presents rational methods for obtaining N-unsubstituted aminonitroimidazoles, which are of practical interest as an intermediate for the synthesis of halogen, diazo-, azido, 1-alkyl-aminonitroimidazoles, triazines. Studies have been conducted to determine the optimal conditions for the synthesis of nitroimidazoles.

The new ways of 4-nitrofurazanilpropancarboxylic acid synthesis

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Keywords: 4-nitrofurazanilpropancarboxylic acid; hydrolysis; synthesis.

4-nitrofurazanilpropancarboxylic acid is initial compound of many energy-saturated compounds synthesis: components of powders, fuels and special-purpose compounds. In this regard, the development of a rational way of obtaining this product is of great importance. Thus, we have developed an alternative method of obtaining a new biologically active substance. The physicochemical properties of the acid obtained by two independent methods completely coincide, including the IR and NMR spectra.

Research on the novel group of explosive d-block metal complexes with tetrazoles – syntheses and properties

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Keywords: tetrazoles; d-block metal complexes.

Polynitrogen organic ligands are of interest to coordinating chemistry, as they have found, in spite of a short period of research, a very wide application. In this group of compounds, tetrazoles and their derivatives have attracted special attention for over a decade. 5-arylotrazoles contain highly electron-deficient aromatic rings, resulting in high electron affinity. Coordination to the metallic center allows to obtain more structurally advanced compounds and contributes to the increase of thermal stability of the tetrazoles themselves.

The mechanism of formation of coordination compounds based on tetrazolium ligands, as well as the formation of tetrazoles from the CN^- and N_3$^-$groups on the metallic center are not well researched and described. What is more, the number of known complexes with tetrazoles is relatively small. Therefore, an attempt to research these issues is a valuable contribution to the development of diverse high-energy materials.

In the reaction of tetrazoles: 2-(1H-Tetrazol-5-yl)phenol, 4-bromo and 4-chloro-2-(2H-tetrazol-5-yl)phenol with vanadyl acetylacetonate (IV) and in the reaction of 5-(3-Pyridyl)-1H-tetrazoles with K_3Na[Mo(CN)_4O_2]·6H_2O new complexes were obtained. In the next step, the physicochemical properties of the obtained complexes were determined, including their thermal stability. Thermogravimetric studies and DSC were used in the study of durability and to determine parameters such as thermal decomposition processes and explosion temperature.

Evaluation of thermodynamic parameters of low-gaseous pyrolants

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Keywords: low-gaseous pyrolants; metal additives.

Thermodynamic analysis of combustion parameters of low-gaseous pyrolants is performed. Two reactive oxidizers of potassium perchlorate (KP, KClO4) and potassium nitrate (KN, KNO3) are considered. Zirconium (Zr) and boron (B) are considered as high energetic metal fuels. Temperature and energetic effectiveness of cross-linked mixtures of KP/Zr KP/B and KN/Zr KN/B are investigated. Zirconium is considered as an additive leading to remarkable high temperature of products, in comparison to other metallic components. In particular, relevancy between heat generation and amounts of gaseous and condensed phase products is inspected. Thermodynamic evaluations are performed with MWEQ[2] program package that in particular is able to evaluate of chemical substances that are present in the reactive mixture in trace concentrations. Several components in condensed (state or fluid) phases may be acquainted simultaneously. The paper is intended to interpret base effects that appear by changing/rising addition of metal fuels to inorganic oxidizers.

Achievements and actual tasks of the development of detonation synthesis of nanodiamonds

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Keywords: detonation; synthesis; nanodiamond; properties; technology; production.

Results of researches on detonation synthesis of nanodiamonds (ND) were reported at the international conference (Pardubice, 1988). The Russian scientists found formation of ND from carbon of molecules of explosives in 1982. Since this time purposeful researches were conducted on studying of the mechanism of synthesis and physical and chemical properties of the ND. For more than 35-year period the technology of synthesis and enrichment of ND is developed, the automated production is created, and the fields of their rational use in science and technology are found. Modern tasks of further development of detonation synthesis are formulated.

Optical fiber metrology for detonation velocity measurements

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Keywords: detonation metrology; optical fibers.

Small explosive samples, more and more, are used due to the limited quantity of raw materials in research and development projects. Detonation velocity is the most used parameter to characterize the process of detonation front propagation. Many methods based on electrical or optical phenomena have been developed. Most of them need very expensive apparatus, hard to calibrate or to synchronize. The less intrusive and precise are optical methods based on fast streak cameras, or using optical fibers connected to fast opto-electrical converters. The optical methods have the advantage that can be used under magnetic fields. This work presents a new handled and cheap technique based in optical fibers connected to an opto-electronic converter and to a digital recording system. This technique was developed and characterized in two metrological configurations: (1) measuring and recording the rising emitting light (REL) from thermal radiation of the detonation front; (2) measuring and recording extinguishment of laser light (ELL), conducted by the fibers before the cut event, generated by the detonation or shock propagation in optical media. Correlating gap distances and delay times in two or more fibers, placed in parallel positions, is the most used configuration. These metrological configurations were used to calculate the detonation velocity of small PBX samples (seismoplast) with good precision. The last method presents the advantage of the recorded signal can be independent of detonation self radiative process and allows the measurement of shock wave propagation in an inert material The experimental results for detonation front velocity were obtained with a resolution of 0.5 to 2%, for both configurations (conjugated, or not, in one single test). This study opens a way to apply this technique in the ELL mode, for measuring the pressure induced in an inert target by the detonation wave, as well as to characterize the copper cylinder test.

Continuous microfluidic process for formation of ADN-prills

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Keywords: microfluidics; ADN; droplet generator; oxidizer.

Ammonium dinitramide (ADN) has the potential to substitute ammonium perchlorate (AP) as oxidizer in solid propellants, which would avoid the environmental, safety and health issues that AP causes. For the incorporation in a propellant matrix spherical shapes of ADN are necessary. The continuous producing of spherical ADN (ADN-prills) in microfluidic droplet generators offers the benefit of controlling the size and the size distribution of the prills. To show the feasibility of the process, a proper experimental setup was developed. Different droplet generators were tested and the most suitable was chosen. The influence of flow velocity of the continuous and disperse phase and the concentration of surfactants on the droplet size were investigated.

New mixed heterocycles combining pyrazoles and tetrazoles

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Keywords: pyrazole; tetrazole; energetic material; structure elucidation; sensitivity.

3,5-Bis(tetazol-5-yl)pyrazole and 3,5-bis(tetazol-5-yl)-4-nitropyrazole are two new triheterocyclic compounds. They are synthesized from 3-5-dicyanopyrazoles and sodium azide via [2+3]-cycloaddition. Both are molecules of interest as energetic materials as well as their precursors. Characterization was performed by using IR, NMR (1H, 13C, 14N), mass spectrometry, elemental analysis and thermal analysis (DSC or DTA). Crystal structures were obtained by low temperature single crystal X-ray diffraction. Impact, friction and ESD values were determined according to standard methods. The energetic performance of these new triheterocyclic compounds was calculated using X ray densities, heats of formation and the EXPLO5 code and finally compared to each other.

Application of long term stored single and double base propellants in advanced blasting methods for dimensional stone extraction

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Keywords: non-detonating blasting cartridge; single base propellant; double base propellant.

It was investigated the production of low explosive non-detonating mixtures from long term stored single and double base propellants (S and DBP) and ammonium nitrate prills in different configurations. The adhesive coating was made from DBP, dissolved in acetone. The samples of different cartridge casings, filled with non-detonating propellant mixtures was investigated by two methods for velocity of propagation. The applied SBP were with different time of storage. The blasting cartridges were made from the investigated materials and were examined on field tests. The prices of these cartridges were calculated. General information on dimensional stones is presented and its overall information about involved explosives is discussed. The technology and mechanization of extraction and processing of ornamental stones around the World are described. Definitions of special concepts such as 'velocity of detonation' and 'deflagration' are given. The term 'dimension stone' is defined and its main parameters considered.

The new promising test procedure suitable for the energetic materials sensitivity testing

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Keywords: DDNP; Bruceton staircase; Probit analysis; statistical methods; sensitivity to friction.

Paper describes a comparison of the two well-known and well established statistical methods with the newly developed testing procedure. The standardized BAM friction sensitivity test is used for comparison of sensitivity data. The first used method is Bruceton staircase, also called "UP and DOWN". The result of the Bruceton staircase method is value of F50 point. The second used method is probit analysis. The result of the probit analysis is the complete sensitivity curve. The newly developed method is a modified Neyer's sensitivity D-optimal test method. The parameters of the sensitivity curve are continuously estimated using maximum likelihood algorithm. The newly tested algorithm differs from the Neyer´s method by altering the way next level suggestion based on the all previous stimulus levels. The friction sensitivity test was carried out with the selected primary explosive and pyrotechnic mixture. Comparison of the materials sensitivity obtained by the mentioned testing procedures is provided. It was found the main advantage of the new method is time and cost effectivity. Moreover it require less sample counts while providing a maximum statistical data in the form of complete sensitivity curve. Another advantage of the new method is its independence on the beforehand knowledge of the real value of stimulus level.

Tracking the thermal output of plastic explosives with nanosized aluminium

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Keywords: plastic explosive; thermal output; detonation velocity; optical pyrometer; calorimeter; thermal imaging.

In this research, the effect of aluminium nanoparticles as a fuel component of plastic explosives was observed regarding the thermal output and velocity of detonation. Three explosive compositions were prepared based on penthrite, poly(propylene glycol), aluminium and a small amount of ammonium perchlorate (in order to enhance oxygen balance). For the comparison, one composition contained only micron-sized particles of aluminium, and in the other two, micron-sized aluminium was partly replaced by nano-sized. In one composition 30% of total aluminium was replaced by spherical nano-sized aluminium particles (70 nm) and in the other composition, 10% of the total aluminium was replaced by nano-sized. Aluminium nanoparticles morphology and size were observed by scanning electron microscope (SEM) and the obtained images were analyzed in programme Image Pro Plus. The velocity of detonation was measured using system consisted of a photodetector with optical probes, electronic counter Pendulum CNT-91, and a digital oscilloscope. The thermal effect of detonations was tracked using two-color high-speed optical pyrometer and a thermal imaging camera. The energetic potential of the prepared explosives was determined in isoperibolic calorimeter IKA 2000, in the nitrogen atmosphere.

Combustion behavior and thermal decomposition of novel oxygen-rich furazantriazoles

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Keywords: decomposition kinetics; combustion; trinitromethyl; furazantriazoles.

Physico-chemical properties such as combustion behavior and thermal decomposition of 3-nitro-4-[1-(trinitromethyl)-1H-1,2,4-triazol-3-yl]furazan (1) and 3-[(1-fluorodinitromethyl)-1H-1,2,4-triazol-3-yl]-4-nitrofurazan (2), 3,3'-azo-4,4'-bis-[1-(trinitromethyl)-1H-1,2,4-triazol-3-yl]furazan (3), which may have potential use as explosive and propellant ingredient, has been studied. It has been found that the stability of N-trinitromethyltriazoles is relatively higher than stability of similar C-trinitromethylheterocycles. The rate constants of compound 1, obtained under isothermal and non-isothermal conditions, are well described by a single equation in a wide temperature range of 110-182°C with an activation energy of 129.5 kJ/mol. The replacement of one nitro group in the trinitromethyl substituent with fluorine leads to a marked increase in the thermostability of compound 2, while the activation energy increases to 143-153 kJ/mol. An analysis of thermocouple data shows that the burning rate of furazantriazoles 2 and 3 depends on the rate of heat release in the condensed phase. The increased stability of the fluorodinitromethyl compound 2 causes a decrease in the depth of its decomposition in the melt and shifts the leading reaction of its combustion into the gas phase. So it is shown that compound 2 burns by the mechanism of volatile explosives, and combustion of compounds 1 and 3 corresponds to a mechanism with a leading reaction in the condensed phase.

Reduced sensitivity RDX, HMX and PETN crystallized from propylene carbonate in a presence of stearic acid

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Keywords: RDX; HMX; PETN; propylene carbonate; stearic acid.

Energetic materials were crystallized from propylene carbonate solutions with different additives. From tested additives, stearic acid causes formation of more spherical and less defect crystal materials. Obtained reduced sensitivity RDX was less impact sensitive in comparison with starting material (7.5 J and 15 J resp.) and also less friction sensitive (110 N starting RDX, 160 N crystallized). HMX and PETN were also less sensitive and nearly without internal defects and inclusions. Remaining stearic acid in crystal material (0.05 - 0.1%) doesn't change stability parameters and melting point of obtained safer explosives. The advantage of propylene carbonate as a solvent is low price, nontoxic nature and low volatility making crystallization process much safer. Propylene carbonate doesn't form combustible vapours to a temperature 130°C. Solutions can be used more than 30 times.

Preparation and characterization of energetic salts of 5-amino-PATO (AmPATO)

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Keywords: 3,5-diamino-1,2,4-triazole derivatives; nitrocompounds; picryl; 2,4,6-trinitrophenyl; energetic salts; thermostable; high energy; synthesis; X-ray diffraction; properties.

Synthesis and properties of some 3-picrylamino-1,2,4-triazolyl-5-amino salts (AmPATO) are described. A detailed structure of one of the obtained salt, 5-amino-3-[(2,4,6-trinitrophenyl)amino]-1H-1,2,4-triazol-4-ium perchlorate (AmPATOxHClO4) was characterized using low temperature (173 K) single crystal X-ray diffraction: orthorhombic yellow block, space group 'Pbc21', a = 8.6943(2), b = 9.3561(2), c = 17.9963(4) Å, α = 90°, β = 90°, γ = 90°, V = 1463.90(6) Å3, Z = 4, wR2 = 0.0859, R1 = 0.0325; GooF = 1.023, experimental crystal density 1.863 (at 173K) and 1.840 g/cm3 (picnom.) at 293 K. The AmPATO salts were characterized by spectroscopical methods and thermal analysis. Preliminary computer calculated energetic characteristics show that synthesized salts possess an increased energetic characteristics, superior in comparison to the TNT. The AmPATO salts can be interesting as a thermostable high energy materials.

Formulations of different fuel grains for hybrid rocket motor system

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Keywords: hybrid; grain; polymer.

In this work,some fuel grain formulations for hybrid rocket motor are presented. The choise for combustible materials are related to their thermal properties, their calorific power and the ease of forming the hollow cylinder shape of the fuel grain. Polywax, polyethylene, polyurethane and polylactic acid is used as a matrix which is doped with both organic and inorganic particles. We aim to develop and test a new configuration of hybrid rocket motor that will use state of the art solutions. In order to mitigate the shortcomings related to low regression rate and the combustion instabilities, our rocket motor will use a new type of inhomogeneous fuel grain made of two layers of PE paraffin wax doped with metal particles. Also, the combustion parameters will be controlled using an innovative system of real-time sensors mounted inside the chamber. Compared to classic paraffin wax, the PE wax we intend to use has a superior melting temperature, thus preventing the fuel grain to liquefy and collapse inside the chamber. This will be the choice for the inner fuel grain layer, when the mass flux rate can be easily sustained, and another, metal particle doped paraffin wax outer layer, enhancing the regression rate when the interior section of the fuel grain becomes considerably large and the ratio oxidizer to fuel becomes overbalanced. One distinct advantage of using paraffin wax is that can be easily casted when molten. On this property we intend to develop an innovative, two layered, gradient distributed metalized particle fuel grain. This new configuration will be designed in direct relation with the regression rate and will help in achieving constant combustion parameters and uniform thrust. The compensation of the expanding central bore will be made by a rising density of metal particles with the radius. This will be achieved by casting the motor in molten form under centrifugal force. The metallic particles will be micron sized and will be composed of aluminum, magnesium, cooper, etc.

Physicochemical properties of 2,2-dinitro-1,3-bis-nitrooxy-propane

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Keywords: glass temperature; enthalpy of thermal decomposition; 2,2-dinitro-1,3-bis-nitrooxy-propane; constant of thermal decomposition.

Physicochemical properties of 2,2-Dinitro-1,3-Bis-Nitrooxy-Propane (NPN) have been studied. Glass temperature, temperature and enthalpy of thermal decomposition, saturated steam pressure and enthalpy of evaporation as well as thermal stability of 2,2-Dinitro-1,3-Bis-Nitrooxy-Propane have been determined using differential scanning calorimetry and thermogravimetric analysis. Thermodynamic compatibility of NPN with polyurethane, divinylnitrile rubber and polyvinylnitrate have been ascertained.

Special theory of gradual ignition

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Keywords: gradual ignition; propellant.

The poster deals with the contradiction between the geometric law of burning propellant grains and the course of emission functions Γ (livelinesses) measured in the clesed vessels. If the propellant charges burned according to the geometric law, the CV the shapes of the propellant grains would have to distinguish. For example, ball propellant would have to have a high initial and zero final gas emission, while the gas emission of the tubular propellant would initially be smaller, gentle slope and ending at some non-zero value. Instead, the emission functions of powder grains of different shapes are very similar. At the beginning, they often appear "hump" (vzmeryv, klyuv, balooning), then they are carried out approximately according to the geometric law of burning and all ends at zero value. The so-called progressivity of multi-perforated propellants has never been proven. Conversely, the larger the number of channels the propellant grains have, the sooner they fall apart. The poster briefly describes the theory that explains the contradiction between the geometric and physical law of combustion by the phenomenon of gradual ignition of propellant grains. The hydraulic resistance of the propellant grain layer causes the ignition front penetrate the propellant charge at a final rate, and before it reaches the bottom of the shot, the first ignited grains nearest to the igniter have a different dimensions than the last ignited grains. The gradual ignition of the propellant charge has a major impact of the entire course of the ballistic cycle.

Azoles with trinitroalkyl substitution

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Keywords: triazole; tetrazole; trinitroalkyl; X-ray; mechanism.

Some new azoles with trinitroalkyl substitution at nitrogen are presented. The materials were thoroughly characterized using NMR spectroscopy, vibrational analysis, as well as elemental analysis and single crystal X-ray diffraction. Differential thermal analysis (DTA) was used to determine the thermal stability, BAM drophammer and friction tester to determine the sensitivities against impact and friction. The performance parameters of potential energetic compounds were calculated with the EXPLO5 V6.03 computer code based on calculated (X-ray) densities in combination with CBS-4M calculated heats of formation. Mechanistic considerations for the formation of a triazole, which proceeds via nitrosation of an N-substituted diaminomaleonitrile with HNO3 are described.

Modernization of the grinding technology and quality evaluation method cellulose nitrates

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Keywords: cellulose nitrates; grinding technology; conical mill; Kuzmin's disk mill; fractional composition.

The influence of various factors on the quality of fibrous materials grinding was analyzed and the modern method for assessing grinding quality of cellulose nitrates was represented. The results of the physicochemical, structural, molecular properties investigation of cellulose nitrates that are not inferior to the best foreign analogues are given.

A promising energetic compound with excellent detonation performance and low sensitivity

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Keywords: furoxan; 1,2,4-oxadiazole; high detonation performance; low sensitivity,.

Among energetic materials, there is a significant challenge facing researchers: to seek an optimal balance between high performance and safety. By introduction of a novel azo backbone and low-sensitivity C-NO_2 moieties, a promising energetic molecule, 3-(4-nitro-1,2,5-oxadiazole-2-oxide -3-yl)-5-((3-(4-nitroisoxazol-3-yl)-1,2,4-oxadiazol-5-yl)diazenyl)-1,2,4-oxadiazole (6) was prepared and well characterized by IR and multinuclear NMR spectroscopy, elemental analysis, DSC measurement, and single crystal X-ray diffraction. It shows low mechanical sensitivity (IS: 12 J, FS: 180 N), and superior detonation performance (D: 9666 m s^{-1}, P: 42.8 GPa). Furthermore, the detonation test of 6 was conducted. The result indicates that 6 is more powerful than the secondary explosive HMX. The combination of advanced performance and desirable safety make it a potential replacement for the commonly used explosives HMX.

Potassium 5-(dinitromethyl)tetrazolate: a green energetic 3D metal-organic framework (MOF) as a primary explosive with high thermal stability

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Keywords: tetrazole; energetic material; metal-organic framework; primary explosive; crystal structure.

Current lead-based primary explosives are toxic, which have to be replaced. In this study, the ligand 5-(dinitromethylene)-4,5-dihydro-1H-tetrazole was obtained by simple one-step synthesis. And potassium 5-(dinitromethyl)tetrazolate, cosisting of two K ions, a tetrazole moiety and a dinitromethyl group, was synthesized by self-assembly at ambient temperature and pressure and then fully characterized to be a new 3D energetic metal-organic framework (MOF). Its amazing properties such as high density (2.13 g/m^3), high thermal stability (Tdec = 274 °C), sensitivity (IS = 2 J; FS = 5 N), and calculated superior detonation performance (D = 7259 m/s; P = 23.4 GPa), make the new MOF a successfully candidate as a environmentally acceptable primary explosive.

A novel derivatization strategy for FOX-7

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Keywords: FOX-7; chlorination; protection-deprotection; nitrolysis; high energy; insensitivity.

Synthesis of new polynitro 1,3,5-triazacyclohexane energetic compounds deriving from 1,1-diamino-2,2-dinitroethylene (FOX-7) is reported. We used a smart chloride-assisted protection-deprotection strategy for various derivatization reactions of FOX-7. These new compounds exhibited high crystal densities, excellent detonation performances, as well as acceptable impact and friction sensitivities, demonstrating their promise as potential candidates for high-performance HDEMs. Among them, compound 9 (α and β polymorphs), which contain FOX-7 structural fragment in structure, has excellent sensitivity values (IS $\geq$ 20 J, FS $\geq$ 216 N) and exhibits good calculated detonation values comparable to RDX or FOX-7. Compound 10 (9255 m s-1 and 41.1 GPa) exhibits superior detonation properties compared with HMX (9144 m s-1 and 39.2 GPa). This study not only provides a new strategy for synthesizing new FOX-7-derived energetic materials with excellent properties, but also opens a new path to the ever-expanding chemistry of FOX-7.

Catalyzed ammonium perchlorate with nano copper oxide : a new generation of highly energetic composition

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Keywords: Ammonium perchlorate; transmission electron microscopy; scanning electron microscopy; differential scanning calorimetry; X-ray diffraction.

A new generation of advanced highly energetic composition depends on use Nano-sized oxides including CuO. Nano CuO has a wide range of applications in energetic material field due to his large surface area and high surface energy. This manuscript reports on synthesis of nano CuO by a liquid-state reaction method .The obtained nano CuO characterized by scanning electron microscope (SEM), transmission electron microscopy (TEM) and X-ray diffraction (XRD) for particle size, purity and morphology. The effect of nano CuO on the thermal decomposition of AP has been examined by differential scanning calorimetery (DSC). The results showed that the average sizes of the nano-cuo particles which have been prepared are in the range of 10-20 nm. The thermal degradation rate of AP was increased by 23% due to the addition 1% nano-CuO and the amount of heat release increased by 51%. These results have direct effect on the burning behavior, performance and combustion characteristics of the solid rocket propellants.

Thermal behavior of MWCNT/ammonium perchlorate particles

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Keywords: ammonium perchlorate; scanning electron microscopy; X-ray spectrometer; differential scanning calorimetry.

A novel generation of highly advanced energetic systems depends on carbon nanomaterials (CNMs) such as expanded graphite (EG), carbon nanotubes (CNTs), graphene, and graphene oxide (GO). Carbon nanomaterials (CNMs) has a widely used as an energetic storage and catalysis in energetic material field due to his large surface area and high surface energy .One of the most advantage of (CNMs) is using as carriers of energetic components by coating or encapsulation. This study reports on catalyzed ammonium perchlorate (APC) by MWCNT. MWCNTs were effectively encapsulated with APC particles by using modified fast-crash solvent–antisolvent technique and characterized by scanning electron microscope (SEM) and Energy dispersive X-ray spectrometer (EDX). The catalytic performance of MWCNT on the thermal behavior of ammonium perchlorate (APC) was analyzed by using differential scanning calorimetery (DSC) and thermal gravimetric analysis (TGA). Interestingly, effect of MWCNTs on the thermal decomposition of APC where the results shown that encapsulated APC with 1% MWCNT show significant reductions of the high decomposition temperature from 452.8°C of APC to 390.1°C and MWCNTs offered an increase in total heat release of APC by 130 %. The results confirmed that MWCNTs are a novel catalyzing agent on the thermal decomposition of ammonium perchlorate which has a direct effect on the burning behavior, performance and combustion characteristics of the solid rocket propellants.

Synthesis of magnesium oxide nano particles: a novel nano catalyst in solid rocket propulsion systems

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Keywords: catalyst; thermal behavior; transmission electron microscopy; differential scanning calorimetry; X-ray diffraction.

Magnesium oxide nanoparticles have been synthesized by the liquid-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 effect of magnesium oxide nanoparticles against the thermal behavior of AP was tested by differential scanning calorimetery (DSC).The TEM and XRD results showed that the particle size of magnesium oxide nanoparticles was between 20 nm. DSC results shown that the rate of thermal decomposition of AP in the presence of 1% Nano- magnesium oxide increased 18%, which have a direct effect on the burning behaviour of the rocket propulsion systems.

Novel pyrotechnic without bridge based on the carbon fiber composites

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Keywords: bridgeless pyrotechnic; carbon fiber; primary explosive; carbon-based energetic composites.

Carbon-based energetic composites (CEC) is prepared by mixing carbon fibers with lead azide (LA), lead stephanate (LS) and nickel hydrazine azide (NHA) respectively. The relationship between carbon fiber content and performance of the igniters was studied. The experimental result indicated that the ignition voltage of the igniter is the lowest when the carbon fiber content is 30%. The 50% ignition voltage of NHA-CEC igniter, LS-CEC igniter and LA-CEC igniter is 14.1 V, 17.6 V and 27.8 V from high to low, and the corresponding 50% electrostatic ignition voltage is 30 kV, 28.9 kV and 27.3 kV respectively. The ignition process of igniter was investigated by high-speed camera and lead plate test of detonator. The results show that all three ignitors have reliable ignition ability, and especially LA-CEC and NHA-CEC have reliable detonated RDX ability and perforated the lead plate. The bridgeless pyrotechnic used CEC show more anti-electrostatic ability and fabricated easily to the bridge wire and semiconductor bridge pyrotechnic.

Investigation of electrostatic discharge sensitiveness of 4,6-dinitrobenzofuroxane complexes (with selected monovalent metals)

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Keywords: metal complexes; 4,6-dinitrobenzofuroxane; potassium; electrostatic discharge; sensitivity.

Previously was found that potassium 4,6-dinitrobenzofuroxane complexes have a high sensitiveness to electrostatic discharge stimuli and MIE level was measured about 30 μJ. This lead our work to focus also on the other 4,6-dinitrobenzofuroxane complexes with metal monovalent ions. From range of monovalent metal ions beside of potassium, complexes with sodium, rubidium, cesium and silver were prepared and investigated. Combinations with the selected admixtures (i.e. graphite, carbon black, copper powder, etc.) were also investigated on the influence of the ESD sensitiveness. Obtained results indicate high sensitivity of the all of tested complexes. For alkali metal ions MIE levels shows the trend to rise with increasing molecular weight of metal ions. Nevertheless, obtained MIE levels are very low up to 250 μJ. These levels were not affected by using any of the selected admixtures. On the other hand compacting of samples (resp. rising bulk density) resulted in certain cases at considerable increase of minimum initiation energies. Especially in mixtures with graphite compacting resulted in values of minimal initiation energies exceeding levels of 500 μJ. In contrary with the all tested metal ions the silver complex was found to be relatively insensitive to ESD stimuli. Measured MIE of the silver analog is 10 mJ. The influence of the complex cation and used admixtures on the overall ESD sensitiveness is discussed.

Assessment of the REACH influence on energetic materials after the sunset date

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Keywords: restriction; environment.

European Union's Regulation (EC) 1.907/2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) has come to its sunset date for a great number of substances used for military purposes on the 31st May 2018. The ad literam application of the regulation includes interdiction, restriction or authorization of raw materials in a wide variety of munitions and pyrotechnics. The implications are prominent both for industry and research, and the envisaged outcome includes at least short-term restrictions for the institutions of the defense system.

Study on the reaction mechanism of Al-Zn alloy powder in general heated system

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Keywords: alloy fuels; thermal oxidation; metal combustion; energetic materials; gas atomization.

In order to overcome the problems encountered in the application of pure Al fuel, such as incomplete combustion, low burning rate and high ignition temperature. An approach suggested in this work is to design and preparation a new type of metallic-alloy additive——Al-Zn by gas atomization method and the products was characterized by XRD and SEM. The SEM shows that the Al-Zn powder is spherical and has a granular logarithmic normal distribution. Coupled with EDS, it is noticed that the zinc has a desirable distribution in the particles. TG-DSC method studied the oxidation process of Al-Zn powder, compared with the aluminum powder with the same particle size, the oxidation rate was faster, the weight gain was more, and reaction was more complete. Because of the melting point and boiling point of zinc is much lower than aluminum, so it can melt and gasify at a low temperature, causing the auto-explosion of aluminum from the micro level into sub-micron level, thereby improve the combustion rate of Al and increase the energy release rate of energetic materials.

Crystal engineering for creating low sensitivity and highly energetic materials

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Keywords: energetic materials; crystal engineering; energetic cocrystals; energetic ionic salts; systematic theory.

Energy and safety are the two most important concerns of energetic materials (EMs), while they usually contradict with each other: the high energy goes with the low safety together. Low sensitivity and highly energetic materials (LSHEMs) balance well the energy and safety, and thus are highly desired for extensive applications. Nevertheless, wholly, the energy-safety contradiction, the energy and component limits, and the insufficient knowledge about the relationships among components, structures, and properties and performances of EMs, make the LSHEMs, or even the entire EMs, evolved slowly. This Perspective focuses upon the current progress in the clarifications of the energy-safety contradiction and the crystal packing-impact sensitivity relationship of EMs. Also, we propose strategies for creating new LSHEMs or desensitized EMs through crystal engineering, covering traditional EMs composed of neutral single-component molecules, energetic cocrystals and energetic ionic salts. Two levels of intrinsic structures, molecule and crystal, are accounted for constructing LSHEMs: at the molecular level, it is proposed to make much chemical energy stored in bonds while avoid any too weak bond formed in an energetic molecule to intrinsically balance the energy and safety; at the level of crystal, it is suggested to enhance intermolecular interactions to increase packing compactness and energy density, and to strengthen the anisotropy of the intermolecular interactions to facilitate ready shear slide and low mechanical sensitivity; and overall, a big π-bonded energetic molecule with an oxygen balance close to zero and a hydrogen bond-aided face-to-face π-π molecular stacking is preferred to be a LSHEM. Hopefully, this Perspective will set a root for establishing a systematic theory for creating LSHEMs.

Synthesis of two new gem-fluoronitro contained tetranitroadamantanes and property comparison with their nitro and gem-dinitro analoguess

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Keywords: energetic materials; cage compound; tetranitroadamantane; fluorination; oxidative nitration.

Two new fluorinated tetranitroadamantanes, 2,6-difluoro-2,4,4,6-tetranitroadamantane and 2,4,6,8-tetrafluoro-2,4,6,8-tetranitroadamantane, were synthesized. 2,6-Difluoro-2,4,4,6-tetranitroadamantane was prepared from 4,4-dinitroadamantane-2,6-dione by a three-step route with an overall yield of 40%. It has a slightly higher crystal density (1.787 g cm^{-3}) than its analogue 2,2,4,4,6,6-tetranitroadamantane (1.777 g cm^{-3}). 2,4,6,8-Tetrafluoro-2,4,6,8-tetranitroadamantane was prepared from 4,8-dihydroxyadamantane-2,6-dione by an eight-step route with an overall yield of 8%. It is notable that the replacement of one nitro group in gem-dinitro functonality with flluorine might slightly reduce the detonation performance but improve the density and inherent steric hindrance, which makes possibility for introducing more nitro functionalities on the adamantane backbone.

Experimental study and numerical simulation of explosives containing B/Al in underwater explosions

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Keywords: explosion mechanics; explosive containing B/Al; underwater explosion; shock wave; bubble; numerical simulation.

To research the effect of content of Boron/Aluminum (B/Al) compound powder on energy output property of metallized explosives in underwater explosion, three HMX-based explosives containing B/Al (PF-1, PF-2, PF-3) were designed and prepared. The underwater explosion experiments of samples with size of Φ100×105mm were taken, six overpressure sensors were installed at the position of 2m, 3m, 4m, 5m, 6m and 7m away from sample center on one side to measure the shock wave pressure, and two overpressure sensors were installed at the position of 3m and 4m away from sample center on the other side to measure the bubble pulsation period, the shock wave energy, bubble energy and total underwater explosion energy of three kinds of explosives were calculated. In the meantime, the underwater explosion process was simulated by the finite element program AUTODYN. Results show that the shock wave pressure error is less than 5%, and the bubble pulsation period error is less than 6%Among the three kinds of explosives, the maximum bubble energy and total energy is produced by PF-3 charge with 20% content of B/Al compound powder. For the HMX-based explosive containing B/Al, the combustion of Al powder can lead to the combustion of B powder in the condition of explosion according to the combination effect, which will release more combustion heat and improve the total energy of underwater explosion. Moreover, bubble pulsation can improve total energy obviously by taking the advantage of explosive containing B/Al powder in underwater weapons, which has significance for efficiently damage of munitions, and has a prospect for military affairs.

A stepwise strategy for the synthesis of HMX from 3,7-dipropionyl-1,3,5,7-tetraazabicyclo[3.3.1]nonane

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Keywords: 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane; 3,7-dipropionyl-1,3,5,7-tetraazabicyclo[3.3.1]-nonane.

1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane(HMX) is one of the most powerful and widely used explosives. A new method for the synthesis of HMX from 3,7-dipropionyl-1,3,5,7-tetraazabicyclo[3.3.1]nonane (DPPT) was investigated. Two important intermediates, 1,5-dipropionyl-3-nitroso-7-nitro-1,3,5,7-tetraazacyclooctane (DPNNO) and 1,5-dipropionyl-3,7-dinitro-1,3,5,7-tetraazacyclooctane (DPDN), were isolated from the reaction mixture. The reaction mechanism, involving a nitrolysis-nitrosolysis-nitrolysis-nitrolysis process, was proposed and verified by the H-NMR tracking. Based on the reaction mechanism, a stepwise method to prepare HMX from DPPT was developed. DPPT could be efficiently and smoothly converted to DPNNO in red fuming nitric acid with excellent yield up to 94.2%. The influence factors on the yields of HMX such as reaction temperature, loading amounts of N_2O_5 were investigated. Under the optimized conditions, HMX was obtained with a satisfactory yield of 85.0%. The overall yield of the stepwise procedure was as high as 80.0%.

Mechanical response of multi-layer corrugated structure to blast loading

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Keywords: multi-layer corrugated structure; blast load; structural response; energy absorption.

The shock resistant plate is fitted under the vehicle floor, like the V shape plate which is often used for explosion reflecting on the Casspir Armored Personnel Carrier (APC). Wavy structure can change the energy transfer and dissipation process of shock wave by coupling effect among layers, which has excellent properties such as light weight, high specific strength, high specific stiffness, good energy absorption and vibration damping. This paper designed a corrugated structure and simulated the dynamic response of corrugated structure. The newly designed structure consists of three materials: hardened material, shock bumper material and high tenacity material. The impact resistance was studied by comparing the explosion pressure, energy absorption, displacement, velocity, acceleration and strain of the upper and lower layers.

Comparative study on reaction characteristics of micron-sized aluminum and nano-sized aluminum in O_2 and CO_2 environment

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Keywords: reaction characteristics; Al powder; thermal analysis; reaction products.

To understand the difference in reaction behavior of micron/nano Al powder in O2 and CO2 environment at 25-1500 °C, thermal analysis experiment for 50 nm and 1.5 μm Al powder was performed in this study. The experimental results show that the reaction of 50 nm and 1.5 μm Al powders with O2 mainly occurs at 530 – 570 °C and 800 – 1500 °C, respectively. In CO2 environment, the reaction of 50 nm and 1.5 μm Al powders with CO2 mainly occurs at 475 – 900 °C and 600 – 1500 °C, respectively. For reaction products, most of the reaction products condensed together and form agglomerated Al2O3 in O2 environment. However, in CO2 environment, because the oxidation reaction rate and reaction heat between Al and CO2 are lower than that between Al and O2, the particles of the reaction product are still relatively independent. The experimental results clearly show the reaction characteristics of micron/nano Al powder in O2 and CO2 environment, which is of great significance for the study of ignition and combustion mechanism of Al powder.

Keyword Index

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The End