Abstracts of the 18th Seminar on

New Trends in Research of Energetic Materials

Pardubice, April 15–17, 2015

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Institute of Energetic Materials

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New Trends in Research of Energetic Materials

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Preface

This eighteen seminar NTREM takes place in the year of 95th anniversary of the beginning of education in the field of science and technology of explosives in Czechoslovakia; This scientific-pedagogical activity was initiated in 1920 at the Prague Institute of Chemical-Technological Engineering (now Institute of Chemical Technology – VŠCHT Prague). In the same year, Explosia (a company manufacturing explosives) was established at Pardubice. These two events significantly affected the development of energetic materials in Czechoslovakia, which at that time was a young republic, formed in 1918 after disintegration of the Austro-Hungarian Empire. These developments, together with the high standard of the Czech mechanical engineering industry, resulted in Czechoslovakia becoming a significant manufacturer and exporter of weapons, ammunition and explosives before the Second World War. After liberation of Czechoslovakia, the education was rehoused on September 1953 from the Institute of Chemical Technology in Prague to, at that time, the Institute of Chemical Technology in Pardubice (VŠCHT Pardubice). A continuator in this activity in nowadays, Institute of Energetic Materials (IEM), pursues its pedagogical, research and scientific activities as a constituent part the Faculty of chemical technology [1]. It provides education in master's or doctoral's programs in Physics of Explosion, Chemistry and Technology of Individual Energetic Materials, Technology of Explosives and Safety Engineering which are open for domestic as well as international students. These programs are available for students pursuing degree in both civil and defense technologies. The Institute is also a center of continuing professional education for specialists dealing with energetic materials, Physics of Explosion, Safety Engineering and mitigation of terrorist threaths. This institute was practically unknown to the World until 1998.

The present-days the Institute of Energetic Materials has happened to be widely known in the World only after starting its activities in the International Seminars NTREM organization [2]. One of the decisive factors enabling realisation of these seminars has been the financial assistance of well-wishers of this activity. Traditionally, the seminars were sponsored by number of institutions enabling attendance of wide range of participants including students and young researchers not yet well financially covered by research grants. For this support we would like to thank all of our sponsors that have decided to support us again this year. Special thanks go to the Office of Naval Research Global - U.S. Navy, Embassy of the USA in, Prague, Austin Detonator Vsetín, Indet Safety Systems (a member of Nippon Kayaku Group) Vsetín, Faculty of Chemical Technology of the University of Pardubice, Explosia Co. Pardubice, OZM Research Hrochův Týnec, Institute of Shock Physics at London Imperial College, Nicolet, Prague. The efficient help in ensuring smooth and successful course of the meeting obtained from all these institutions is gratefully acknowledged. We greatly appreciate that thanks to this support all the specifics of the seminar can be preserved.

And traditionally, I wish to 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 and its influence on the continued success and growth of all future meetings at our University of young people and university teachers working in the field of teaching, research, development, processing, analysing and application of all kinds of energetic materials.

Allow me to use this opportunity for inviting you in the name of my co-workers and myself: we are looking forward to meet you at the seventh seminar in the second half of April 2016 in the Aula Magna of our University.

[1] S. Zeman, "The Teaching of Explosives Sciences in the Czech Republic Celebrates its 95th Anniversary", *Review, Czech Defence Industry & Security*, 2015, No. 1, 36–37.

[2] S. Zeman, "Teaching of the Chemistry and Technology of Explosives in the Czech Republic". In: R. W. Armstrong, J. M. Short, R. A. Kavetsky, D. K. Anand (Eds.), *Energetics Science and Technology in Central Europe*, Center for Energetic Concepts Development Science, University of Maryland, 2012, pp.1–11.

Pardubice, March 13th, 2015

Svatopluk Zeman

Review of some peculiarities of the stability and decomposition of HNF and ADN

Manfred A. Bohn

Fraunhofer Institut für
Chemische Technologie (ICT)

Keywords: HNF; ADN; stability of HNF; decomposition of HNF; stability of ADN; decomposition of ADN.

HNF (hydrazinium nitroformate) and ADN (ammonium dinitramide) are seen as possible replacements for the common oxidizer ammonium perchlorate (AP) in composite rocket propellants. Both HNF and ADN have the relatively great advantage to be chlorine free. But their chemical stability is much lower than the one of AP. In spite of this they are still on the list as replacement candidates. This paper intends to review and compile essential features in stability, compatibility and decomposition behaviour of the two candidates. HNF alone can be seen as relatively stable at temperatures up to 50°C. But it shows self-accelerating decomposition behaviour. In such a case normally stabilizers help to suppress autocatalytic behaviour as it is possible with nitrate esters. This seems not a way with HNF. A look on possible decomposition behaviour reveals that HNF seems not stabilizable. Further problems are chemical compatibility and a too high pressure exponent of the propellant formulations. ADN can be qualified as medium stable at lower temperatures similar to NC-based products. Also ADN shows self-accelerated decomposition. In contrast to HNF, it can be stabilized and a lot of possibilities exist, some stabilizers are superior. The reason for the stabilisation by stabilisers can be found in the difference in decomposition mechanisms, which will be shown. From the results presented one can conclude that ADN has a perspective to replace AP in propellants designed for selected applications. A 'universal' application as with AP-based composite rocket propellants seems at time not realistic. Special measures as coating of ADN particles may improve the situation with regard to manufacturing and compatibility, but the limited in-service temperature range will be not changed.

Issues affecting safe handling of peroxide explosives

Jimmie Oxley, James Smith, Matthew Porter, Lindsay McLennan, Kevin Colizza

University of Rhode Island

Keywords: HMTD; peroxide explosives; sensitivity; stability.

While the so-called "homemade" explosives are not new, they have been examined and rejected by the military due to their poor stability and high sensitivity, researchers in various aspects of counterterrorism find themselves forced to handle them. The University of Rhode Island has made a study of characterizing such materials for the purpose of documenting their signatures, determining if reasonable ways of inerting them can be found, finding the safest way to handle and destroy them. This talk will feature our studies on HME—mechanistic, gentle destruction, compatibility with various materials. Application of lessons learned in terms of destruction, safe handling and safe methods of providing vapor signature will also be discussed.

Forecast of possibility for practical application of energetic materials

Aleksandr Smirnov, Oleg Voronko, David Lempert, Tatyana S. Pivina

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Keywords: explosives; enthalpy of formation; explosive characteristics; detonation velocity; detonation pressure; relative throwing ability; ballistic parameters; sensitivity.

The analysis of the data on the properties of the "new" explosives has been conducted. The estimations of the properties presented in the references have been considered for a wide range of the explosives from various chemical classes. Among other things, the physical and chemical parameters (the enthalpy of formation and the density of a single crystal) have been considered and the calculation of the explosive characteristics (the detonation velocity & pressure, the heat of explosion, the relative throwing ability, the impact & friction sensitivity) and the ballistic parameters (pulse) has been executed. It is shown, that for some of the explosives in the references highly overestimated evaluations of the values of the enthalpy of formation resulting in the big error at forecasting of the basic parameters of action have been reported. For some of the most promising explosives, the calculation of the properties of the explosive compositions and the composite propellants on their basis has been carried out: the detonation velocity and pressure, the heat of explosion, the relative throwing ability, the air explosion pressure and pulse, the shock sensitivity, the thrust pulse. The optimization of the component composition according to the parameters of the power and safety has been conducted. The conclusions on the dominating requirements to the energetic materials offered for the replacement of the nominal ones has been drawn.

The effects of first-stage detonation-propulsion on shaped charge jet break-up

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Keywords: explosives; detonation; shaped charge jet; break-up; modelling.

This paper's goal is to reveal to students and young researchers how initial brisant coupling from condensed explosive affects a shaped charge's liner material so as to affect break-up of its jet into particles. The paper reveals topical areas that can be more thoroughly examined by them by means of new experimental work on condensed explosives, their detonation and their modeling.

Shaped charge jet break-up is usually studied as a function of initial liner material properties and modeled under assumptions regarding material heating, strain, and strain-rate. Most jet break-up models, such as those using Hirsch's Vpl factor, relate a yield-stress related term to a velocity related term where these are used either to describe local conditions along the jet or with respect to initial parameters: explosive composition, liner material, and device design and manufacture. Work presented at NTREM 2007 revealed that when these initial parameters were held constant in a shaped charge experiment series while the liner thickness was changed, then Vpl had to be changed in three different modeling codes – Vpl increasing as liner thickness increased. This finding implied that explosive-to-metal coupling during first-stage propulsion was affecting the propelled material differently; and an apparent relationship describing this was developed from first-stage propulsion formulas presented at NTREM 2006. Improved first-stage propulsion formulas were presented at NTREM 2008 and 2011.

The proposed paper and presentation reveal that the improved formulas show that initial brisant coupling has varied along the liner in all previous shaped charge work as a result of device design with the result that the propelled liner was affected differently along its length and thus also differently along the stretching jet. In other words, the liner's material properties were affected in a non-uniform manner that violated major assumptions in previous jet break-up modeling. Evidence supporting this finding will be drawn from historical scientific literature adding to citations used at NTREM 2007 as well as from additional examples in high-speed photography and flash radiography.

Experiment and numerical simulation research on the JO-9c micro-charge detonation growth rules

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Keywords: micro charge; detonation growth; manganin piezo-resistance method; numerical simulation.

In order to study the micro charge detonation growth rules, a method through experimental tests in combination with numerical simulation was used to measure the detonation pressure under different heights. The detonation pressure is accurately obtained by manganin piezo-resistance method to get the fitting curves and expressions of detonation characteristics about micro-charged JO-9c with two different charge densities. The commercial software AUTODYN was employed to simulate the non-ideal detonation process described by the ignition and growth model. The obtained pressure was compared with experimental data. The results show that the deviation between the numerical simulation data and the experimental values is within 15%, indicating that numerical simulation method can be used to study micro charge detonation growth process. There exists an obvious detonation growth process with a diameter of 1.88 mm. Within the height of 1 4 mm, the detonation grows significantly; while more than 4 mm, the detonation growth trends towards sufficient stability.

Spherical deterred propellant: Influence of the initial temperature and ageing on the mechanical integrity

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Keywords: mechanical integrity; firing temperature; gun propellant; ageing; ballistic firing; closed vessel tests; impact tests.

Initial temperature and ageing play an important role on the ballistic properties of gun propellants. Both are key factor for accuracy and safety. Besides an effect on ballistic properties of gun propellants, initial temperature and ageing has an effect on the mechanical integrity of the propellant particles. The effect of initial temperature and ageing on mechanical integrity has been investigated for a spherical deterred propellant. The propellants have been conditioned at temperatures ranging from -54°C to 71°C. The mechanical integrity of the propellant particles has been determined by a quasi-static compression of a propellant bed and subsequent firing of the previously pressed grains in a closed vessel. It has been observed that the mechanical integrity changes hardly with ageing at 71°C and 21°C. At low temperatures (-20°C and -54°C), significant change of mechanical integrity of the propellant particles as a function of ageing time is noticed. Additionally, microscopy observations and impact tests of the pressed grains propellant have been done.

High speed thermography measurements on intermetallics

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Keywords: intermetallics; temperature measurement.

A number of plate impact experiments were conducted as part of a collaboration between the University of Cambridge, LEME (University of Paris X) and QinetiQ to measure the temperature of intermetallic reactions. The results of these experiments, on powdered nickel and aluminium showed a clear threshold for the onset of reaction and subsequent increases in temperature observed with increasing impact velocity. Such data give an insight into the kinetics and reaction mechanism of the materials concerned.

Catalyst action mechanism on low-calorie propellant combustion

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Keywords: propellant; combustion; catalysts; electron microscopy; X-ray analysis; electron probe analysis.

Prevously was found that lead-copper catalysts are effective only in the presence of carbon frame on the combustion surface where substantional accumulation of catalysts is taken place. Herewith the leading burning zone is above the combustion surface. It is also known that this kind of additives are slightly affect on the low-calorie propellant burning. The reasons for this are not clear, because the possibility of formation of carbon frame on the combustion surface increases with the calorie reduction of propellant. For this kind of propellants iron and nickel catalysts are effective. Nickel-lead phthalate is also increases burning rate of the low-calorie propellant. But mechanism of its action has not been studied. Purpose of this work is to study the processes on the combustion surface of the low-calorie propellant using the copper-lead and nickel-lead phthalates as catalysts with use of electon microsope and X-ray electron probe analysis. Size of catalyst particles is about 5 micron. Catalytic action of additives was conducted during the combustion of two propellants with Q_l = 2151 kJ/kg and Q_l = 2518 kJ/kg. Various amount of catalysts was added in excess of 100% into the propellant as individual and also in aggregate with carbon black.

Environmental impact of an emulsion explosive in a life-cycle perspective

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Keywords: life-cycle assessment; civil explosives; environmental impact; energy requirement.

To reduce the environmental impacts of civil explosives, it is essential to adopt a life-cycle perspective. The main goal of this article is to present a comprehensive Life-Cycle Assessment of a civil explosive production and use in order to identify the life-cycle phases with lower impacts and opportunities for improvement. The selected explosive was an emulsion explosive. A detailed inventory for the production was implemented, based on data collected from a specific European company. For the use phase, it was compiled data from literature with information regarding the amount of explosives used and also the inherent emissions associated with the detonation. It was defined two functional units for which all the impacts are related: 1 kg of TNT equivalent for the production phase and 1 m3 of rock extracted for the use phase. Two complementary Life-Cycle Impact Assessment (LCIA) methods were used to assess primary energy requirement (CED method) and six environmental impacts (CML method). The results showed that production phase have a higher contribution to the impacts compared to the use phase. The main contributor to the production phase, for the seven impact categories, is the emulsion explosive composition, ranging from 82% (Photochemical Oxidation) to 96% (Eutrophication) mainly due to ammonium nitrate production.

Study of the thermal decomposition of PGDN

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Keywords: PGDN; thermal decomposition; vapor pressure; duality DSC-TGMS.

Propylene Glycol Dinitrate (PGDN) is a liquid nitroester explosive which has been used as gelatinous agent in some energetic formulations. In this work, PGDN has been synthesized and characterized in order to study its thermal decomposition. The PGDN is first characterized by gas chromatography-mass spectroscopy (GCMS), and Fourier transformed infrared spectroscopy (FTIR). Differential scanning calorimetry (DSC) is used for the calculation of the energy of activation and heat of decomposition using two models, Ozawa and Kissinger. The study of the thermal decomposition of PGDN is carried out by using both DSC and thermogravimetry-mass spectroscopy analysis (TGMS) methods. The gases produced during the thermal decomposition are identified by mass spectrometry and the influence of the heating rate is investigated. The duality DSC-TGA is brought out by studying the complementarity between those methods. The vapor pressure and enthalpy of vaporisation of PGDN are estimated using TGA by taking benzoic acid as reference. Langmuir equation and Clausius–Clapeyron expressions have been used, respectively. The result is compared to the other explosives (Nitrolycerin, EGDN. . . etc.) in order to situate the use of PGDN as tagging agent for potential explosive detection.

Extensive theoretical studies on two new members of the FOX-7 family as energetic compounds

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Keywords: DFT; 5-(dinitromethylene)-1,4-dinitramino-tetrazole (DNAT); 1,1'-dinitro-4,4'-diamino-5,5' bitetrazole (DNABT); enthalpy of formation; detonation.

Two novel compounds 5-(dinitromethylene)-1,4-dinitramino-Tetrazole (DNAT) and 1,1'-dinitro-4,4'-diamino-5,5'-Bitetrazole (DNABT) were suggested to be potential candidate of high energy density materials (HEDM). The optimized geometry and electronic density, HOMO-LUMO orbital, electrostatic potential on surface of molecule, IR spectrum and thermochemical parameters were calculated for inspecting the electronic structure properties with B3LYP/6-311++G** level of theory. Meanwhile, the solid state of DNAT and DNABT were studied using the crystal packing models with the plane-wave periodic local-density approximation density functional theory. Four stable polymorphous cells have been found including P212121, P21/C, P-1 and PBCA, assigned to the orthorhombic, monoclinic and triclinic lattice systems. In addition, properties such as density, enthalpy of formation and detonation performance have been also predicted. As a result, the detonation velocity and pressure of two compounds are very remarkable (DNAT: D = 9.17 km/s, P = 39.23 GPa; DNABT: D = 9.53 km/s, P = 40.92 GPa). Considering the tetrazole rings with energetic groups and the insensitive fragment of FOX-7, high positive heat of formation (583.50 kJ/mol and 1081.39 kJ/mol) and eminent performance, render DNAT and DNABT to be very promising powerful energetic insensitive compounds. This work provides the theoretical support for further experimental synthesis.

Resonant acoustic mixing and its applications to energetic materials

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Keywords: resonant acoustic mixing; energetic materials; particle coating; co-crystals; co-crystallisation; RAM; soft mixing.

Resonant Acoustic Mixing (RAM) is a technology developed by ResoDyn Corporation which provides a low-energy contactless mixing system. This paper examines how the RAM technology can be applied to the processing of energetic materials and provides a comparison with conventional mixing techniques. Through research carried out to date, it has been established that RAM technology offers several advantages over traditional mixing techniques, especially where energetic materials are concerned. The main advantage lies in the relatively gentle mechanism of the RAM technique, where only minor damage occurs to sample particulates, with no blades or impellers being used in the process. The extent of particle damage encountered has been assessed by scanning electron microscopy, and shown that very little shear occurs during mixing at low accelerations. The process is also relatively thermally benign, although some temperature excursions have been encountered. Work has been undertaken to prepare energetic co-crystals and salts using a solvent-drop approach in the RAM, offering advantages in terms of diverse container compatibility and fast processing time.

In-situ thermal research on phase diagrams of mixture from ammonium nitrate and hexamethylenetetramine

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Keywords: in-situ; ammonium nitrate; hexamethylenetetramine; urotropine; X-ray powder diffraction.

Mixtures from ammonium nitrate (AN) and hexamethylenetetramine (HMTA) in different proportions were used as explosives in some blast incidents. In this work mixture made from AN and HMTA in proportion 90:10 has been characterized in order to study phase diagrams during its thermal decomposition. The characterization is performed by X-ray powder diffraction (XRPD) using in situ thermal method after heating in the range from 100 ^{o}C to 200 ^{o}C. The influence of the heating rate is investigated.

Further studies on a new stabilizer for nitrocellulose

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Keywords: stabilizer; nitrocellulose; propellant.

Nitrocellulose (NC) based propellants continuously decompose during its lifetime and the degradation products released in this process have an accelerating effect of the decomposition. Therefore stabilizers are added to NC/NG propellants to inhibit these autocatalytic reactions and to maintain high quality of the products during their recommended lifetime. The stabilizers trap the nitrous gases formed in the decomposition of the propellant and form stable compounds, thereby preventing or delaying the autocatalytic process. The state of the art stabilizers such as diphenylamine, Centralites and Akardites all contain an aromatic amine or amide motif, which are prone to form N-nitrosoamines when they react with the decomposition products from the propellant and at least some of these compounds are known to be carcinogenic. Due the health concerns regarding N-nitrosoamines there is a need to develop less toxic and improved stabilizers. In previous work, it has been shown that di(2,6-dimethoxyphenol) ethylene glycol ether also known as Stab-5, has promising stabilizing properties. This stabilizer has showed more than 100 year stability of propellant paste in accelerated aging microcalorimetry experiments performed according to STANAG 4582. In the continuation of the earlier work, identification of degradation products have been performed to initiate investigations regarding toxicity of products formed in the stabilization process. The findings from the investigation showed mono-nitration of the aromatic rings in the 3- or 4-position with an otherwise intact stabilizer structure both under conventional nitration reaction conditions and during long term storage of a real NC/NG ball propellant. In addition to identification of degradation products, a scale up of the process to 500 g scale has been performed with successful outcome. This material will be used in motor testing at Eurenco-Bofors to characterize the mechanical behavior and the burning rate properties of the propellant.

NTO-based melt-cast insensitive compositions

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Keywords: NTO insensitive explosives melt-cast explosives.

The paper presents research on insensitive melt-cast explosive compositions based on 3-nitro-1,2,4-triazol-5-one (NTO) and containing TNT, wax, Al and RDX. The viscosity of the compositions in operating temperature range was measured. Thermal analysis was performed and thermal stability and sensitivity to mechanical and thermal stimuli were tested. Detonation parameters were also determined. Key words: NTO, insensitive explosives, melt-cast explosives

The main principles of the creation of solid composite propellants with high specific impulse but low combustion temperature

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Keywords: specific impulse; combustion temperature; element content.

The dependence of specific impulse and combustion temperature upon enthalpy of formation and element content of the formulation (basing on C,H,N,O atoms only) of solid composite propellant has been investigated for the searching of compositions with combustion temperatures below the predetermined limit, but with maximally high specific impulse. Quantitative relationships linking the above parameters are obtained. It is shown that there is a passage in the region of existence of the compositions satisfying the requirements set to the combustion temperature and specific impulse. The obtained data allow to determine the possibility of creating compositions with desired values of specific impulse while limiting the combustion temperature

Energetic properties of semicarbazidium 4,4',5,5'-tetranitro-2,2'-biimidazolate

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Keywords: TNBI; energetic salts; high-nitrogen compounds.

High-energetic salts of explosives which can form ionic compounds could have more advantages than classic explosives. Cations and anions with high nitrogen content cause improvement in density, standard enthalpy of formation and oxygen balance. During decompositions of these compounds large amount of gaseous products are formed. For that reasons the salts could be introduced to many civilian and military applications. An example of such material is semicarbazidium 4,4',5,5'-tetranitro-2,2'-biimidazolate. The salt can be easily prepared from widely available substrates. After filtration and drying, it shows no signs of hygroscopicity and decomposes at 187°C. The structure of newly obtained compound was confirmed with NMR spectroscopy. Thermal properties were investigated with DTA/TG analysis. We also determined standard enthalpy of formation. Detonation parameters were calculated with Cheetah code for density determined for pressed sample. Detonation ability and velocity of detonation was measured experimentally.

A review of energetic co-crystals

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Keywords: co-crystals; solvates; review.

Developments in energetic materials are currently focused on the requirements for safer, yet still powerful materials for uses within mining, munitions and rocket propulsion systems. One strategy that can be used to achieve these desirable properties is to synthesise new molecules, but this is both time-consuming and resource-intensive. Instead, another strategy is to crystallise energetic molecules with other molecules to form solvates or co-crystals. This approach has been used extensively within the pharmaceutical industry in order to enhance desirable properties, e.g. solubility and bioavailability. To date, however, there has been a lack of research on the co-crystallisation of energetic materials. Examples include trinitrotoluene (TNT) with trinitrobenzene (TNB) or 1, 3, 5-tris (4′-aminophenyl) benzene (TAPB). To start this design process, the relationships between the types and strengths of interactions within a crystal structure and materials properties need to be established. Once these structure-property relationships have been established, the engineering of new and improved energetic materials can be achieved. The main focus of this work is to provide a survey of published energetic co-crystals and their structure-property relationships.

Universal concept of the unique magneto-dipole holographic spectrum of the energetic materials reactionary zones

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Keywords: throttleable small-scale propulsion systems; micro-scale combustion; reaction zones; unique holographic spectrum; resonance spectrum of the reactionary zone; laser-induced excitation.

Fundamental understanding of the micro-scale combustion mechanisms is very essential to the development of the small-scale propulsion systems of the orbital maneuvering vehicles with ability to actively throttle. 3-D micro/nano-scale structures in the reactionary zones is the platform for effective control by combustion processes of the energetic materials at macro-level. The macro-scale phenomena at the energetic materials combustion is result of self-synchronization of the 3-D micro/nano-scale structures of the reactionary zones. Motivated excitation source of the 3-D micro/nano-scale physical structures in the reactionary zones are the micro/nano-scale structures of the electro-magnetic fields. According to our challenging hypothesis, each energetic material has a unique interactive magneto-dipole (electromagnetic) holographic spectrum of the reactionary zone which is the synergetic oscillatory system. Such synergetic system also can be characterized by the frequency code. Our hypothesis is supported by the recent data, obtained in the various model combustion systems. Magneto-dipole 3-D micro/nano-scale structures can be considered as information medium which characterizes the reactionary zone of the energetic material. Instead of using laser-assisted combustion (laser heating of the solid propellant surface) where thrust is variable by adjusting laser power, we suggest excitation of the resonance spectrums of the reactionary zones by means of polarized (resonance) laser radiation. In the paper the phenomenon of laser-induced excitation of the periodic micro/nano-scale structures in the reactionary zones is considered. Additional effects can be obtained by laser-induced self-organizing of the micro/nano-scale structures in the reactionary zones. Also the techniques of scanning by laser radiation of the unique holographic spectrums of the energetic materials reactionary zones are considered. Laser-induced excitation of the resonance spectrums of the reactionary zones along with re-programming of the magneto-dipole spectrum of the reactionary zones gives the possibility for control by the scale and 3-D localization of the induction and energy-releasing areas and, accordingly, allows control inter-scale interaction in the aerospace propulsion systems. The additional technical result is connected with increase of the energy-release rate in the reactionary zones of the energetic materials. Suggested technology also can be considered as a promising one for re-programming of the magneto-dipole holographic spectrums of the interacting reactionary zones of the aerospace propulsion systems. The suggested concept opens new possibilities for development and micro-scale synthesis of the advanced propulsion materials through programming by the magneto-dipole holographic spectrum of the reactionary zones.

The boron particles agglomeration study during the high-energy composition combustion

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Keywords: energetic condensed systems; agglomeration; boron.

Boron is a promising component of energetic condensed systems due to its high gravimetric heat value, which are significantly higher than that of aluminum. However, practical difficulties of the boron particles combustion limit the use of boron because of the liquid boron oxide layer formation with a relatively high boiling point of 2250°C that limits the oxidation of active boron. In the present work, the boron particles agglomeration and the framework (slag) formation processes during combustion of the high-energy compositions were investigated. The quench particle collection bomb technique was used to collect the condensed combustion products formed under nitrogen pressures of 4.0 MPa. The formation of a framework was visualized using high-speed video registration (1200 fps) under nitrogen pressures of 0.1-4 MPa. Particle size, morphology and surface structure of collected condensed products were evaluated using laser diffractometry and scanning electron microscopy. The completeness of the metal fuel combustion was determined by chemical analytic technique and confirmed by TG/DSC-analysis. In the experiments, the weight of the collected condensed combustion products was about 30% of the initial sample weight, where 26% belongs to the products collected from the gas phase, and 4% remains in a highly-porous framework. The initial amorphous boron powder contains 1% of boron oxide with the average particle diameter about 1 μm, whereas agglomerated particles, which are collected during combustion, consist of 80% B and 20% B2O3 with the average particle diameter of 5 μm. The burning rate of compositions without binder is three times higher and the diameter of collected agglomerates is ten times higher than that for compositions with binder.

Monitoring of bond-line stresses in case-bonded composite rocket propellants

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Keywords: composite rocket propellant; monitoring; bond-line stress; stress sensor.

In all case-bonded composite rocket propellant (CRP) types and in all case-bonded elastomer-bonded high explosive charges (HEC) so-named bondline stresses occur when the temperature is unequal to the curing temperature, means not equal to the so-named stress free temperature. The stresses or the forces which act as tensile force on the bondline when temperature is decreased can cause de-bonding from the case. Further on the occurring tangential or ring stresses inside the material can lead to cracks inside the material, especially when the strain capability is not sufficient or decreases with ageing. Therefore a method is developed to monitor such stresses. The method enables a prediction-tool for critical loads with respect to failure of the material. Preferably such a method works non-destructively, means the quantities were determined without destruction or firing of the munitions, here rockets and high explosive warheads.

In a first step built-in stress sensors are used to follow the development of stress values during ageing and thermal cycling. The material is a typical composite rocket propellant with HTPB-IPDI binder and AP and Al as solid fillers. The experimental set-up consisting of several small rocket motors equipped with stress sensors is explained. Results of the measurements are presented and discussed. Again to say any other elastomer binder with any other solid filler load are composite materials which suffer from these mechanisms outlined.

Wetting of oxidizer particles by binder and plasticizer molecules - microcalorimetry experiments and computer simulations

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Keywords: computer simulation; microcalorimetry; oxidizer-binder interaction.

Composite rocket propellants (CRP) contain oxidizer particles and fuel particles in an elastomeric binder matrix: The oxidizing agent is mostly ammonium perchlorate and the elastomer is hydroxyl terminated polybutadiene (HTPB) based polyurethane. The components differ widely in terms of crystallinity, thermal expansion behaviour and polarity. Especially, under broad temperature variations insufficient resilience leads to detachment or dewetting of filler material from the binder. The ageing of such material was successfully characterized by DMA (dynamic mechanical analysis) measurements. The loss factor shows characteristic changes in shape and intensity. The shape of the loss factor is also determined by the intermolecular interactions between binder elastomer and filler materials [1, 2, 3]. Also the transitions between non-glassy and glassy states of polymer binders and plasticizers are strongly determined by intermolecular interaction forces [4]. This work intends to contribute to elucidating this aspect:

Molecular dynamics simulations (MD) procedures are employed for a determination of binder-oxidizing agent compatibility. MD is based on the approximation of atoms as point masses and point charges. Iterative solution of classical equations of motion with interatomic forces yields correct structure and energies within simulated volume elements. The procedure uses the crystal structure of the oxidizer and the molecular topology of the elastomer as input parameters, at given temperature and pressure: First, sets of representative crystal surfaces are identified, which are then loaded with a bulk of adsorbate molecules, means binder and plasticizer moelcules. From simulation runs at experimental conditions, the energy of interaction is extracted. Results are compared to those from solution microcalorimetry: This methods provides with the energetic response upon mixing AP powders with uncured HTPB, or plasticising agents as dioctyladipate (DOA), and azido-terminated glycidylazide polymer (GAP-A). Although originally designed for measurement of heats of solution, the setup is used to measure the heat of immersion within saturated solutions.

Synthesis of azide-functionalized hydroxyl-terminated polybutadiene

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Keywords: azide-functionalized hydroxyl-terminated polybutadiene; azide-HTPB; HTPB.

The paper reports the ways to functionalize Hydroxyl-Terminated Polybutadiene (HTPB) by Azide groups to impart energetic properties to the polymer. Two different synthetic approaches were explored to synthesize Azide-Functionalized Hydroxyl-Terminated Polybutadiene (Azide-HTPB). HTPB is a classic prepolymer for the binder system of composite propellants, widely used for the propellant systems of military and space applications. Functionalizing HTPB by attaching different functional groups has gathered good attention by researchers working in the area of high energy materials. Continuing our endeavor to energize HTPB by functionalizing it with explosive functional groups, Azide functionalized HTPB has been synthesized. The functionalized polymer was analyzed for structure confirmation and determination of important properties. Azide-HTPB obtained by Azidation of 10% double bonds of HTPB showed viscosity of 11Pa.s and glass transition temperature of -66°C.

Thermal decomposition of di- and trinitropyrazoles

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Keywords: nitropyrazole; thermal analysis; high-pressure calorimetry; FTIR spectrometry; evolved gases analysis..

Fully nitrated five-membered heterocycles (pyrazoles), polynitropyrazoles in particular, have been actively studied as promising high-energy materials. Polynitropyrazoles have high den-sity and high enthalpy of formation combined with reduced sensitivity to external stimuli. We have studied thermal stability of the first members of high-energy polynitropyrazoles row, i.e., 3,4–dinitropyrazole, 3,5–dinitropyrazole, and 3,4,5-trinitropyrazole, under atmospheric and increased pressures. The use of increased pressure allowed to reduce the influence of evaporation process of 3,5–dinitropyrazole and to determine the temperature and heat effect of its decomposition, which was found to exceed this value for HMX. For the first time evolved gas products were identified for each stage of decomposition. As a result the proba-ble thermal decomposition pathway for the investigated materials was suggested.

Advances in the area of greener munitions

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Keywords: environmental impact; heavy metals; toxicity; energetic materials; munitions.

The paper provides an overview of the lessons learned in Romanian MoD while trying to reduce the environmental impact of the armament systems, in the context of fast changes in legislative, social and technological challenges. Legislative risks and drivers, steps to be followed and relevant aspects regarding available solutions for reducing the environmental impact of munitions are discussed.

Use of a four-liter-autoclave for conducting deflagration tests

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Keywords: deflagration; azodicarboxamide; closed vessel; pressure rise; arising gases.

For the determination of deflagration capability of energetic substances, the test methods according to VDI 2263-1, part 1.6 and UN-Manual, C.1- und C.2-test are used. These methods are suited to evaluate the intrinsic material property deflagration. For evaluation of deflagration behavior in closed systems, for example in production sites, an appropriate test apparatus is missing. Because of this, the BAM Federal Institute for Materials Research and Testing developed a four-liter-autoclave for conducting the deflagration test under isochoric conditions. Deflagration behavior was evaluated under different parameters e. g. pressure and temperature. On the basis of results it can be seen, that the four-liter-autoclave is suited for the determination of deflagration behavior. On the one hand, the same characteristics as in the standard test methods are obtained. On the other hand, there are additional characteristics, like pressure rise and decomposition velocity. On the basis of pressure measurement, the emerging gas volume and the rate of gas evolution, that are used to design protection measures, can be estimated. The measurements are conducted with the deflagrating substance Azodicarboxamide (ADCA). It is concluded that the four-liter-autoclave is a good alternative for conducting deflagration tests.

New energetic aminotriazoles

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Keywords: triazoles; amino; crystal structure; nitrogen-rich.

We report on new aminotriazoles e.g. 4,4',5,5'-tetraamino-3,3'-bi-1,2,4-triazole which can be used as energetic building blocks in the formation of nitrogen-rich energetic salts. These aromatic heterocycles can be synthesized in an inexpensive and feasible way. They were used as cations in metathetical reactions to form new energetic salt. The nitrogen-rich ionic derivatives show superior properties in terms of temperature stability, density and sensitivity towards physical stimuli. The compounds were characterized using low temperature single crystal X-ray diffraction. All compounds were investigated by NMR and vibrational (IR, Raman) spectroscopy, mass spectrometry, elemental analysis and DTA. The sensitivities towards impact, friction and electrical discharge were investigated using BAM standards and a small scale electrostatic discharge tester. The detonation parameters were calculated using the EXPLO5 V6.02 code. Heats of formation were computed by the atomization method based on CBS-4M electronic enthalpies.

Synthesis of trifluoromethyl-substituted N-aryl Poly-1,2,3-triazole derivatives for energetic materials applications

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Keywords: copper; energetic materials; heat of formation; poly triazoles; trifluoromethyl.

Synthesis, characterization, and energetic properties of $-CF_3$ and $-NO_2$ substituted N-aryl-polytriazole derivatives are reported. The molecules are prepared by a reliable Cu-catalyzed [3+2]-cycloaddition between $-CF_3$ substituted aryl azides and alkynes followed by a nitration sequence and also the base promoted nucleophilic displacement of the halo groups by the 1,2,3-triazoles. The compounds are characterized by analytical and spectroscopic methods; the solid state structures of some of the compounds are confirmed by X-ray diffraction techniques. The synthesized materials decompose in the range of 195–308 ^{o}C; these molecules are therefore considered thermally stable energetic materials. Most of the $-CF_3$ and $-NO_2$ groups-bearing aryl triazoles exhibit good densities (1.80 g/cc) and acceptable detonation characteristics (D=7673 m/s; P=25.0 GPa). Some of the fluorine containing polytriazole-bearing compounds showed positive heats of formation (45–400 kJ/mol).

Prediction of the enthalpies of formation of high-nitrogen furazan-based energetic compounds by quantum chemistry

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Keywords: enthalpy of formation; quantum chemistry; energetic compounds.

Important characteristics of explosives and propellants can be calculated from the enthalpy of formation, which is closely related to the stability and sensitivity of these compounds. The experimental enthalpies of formation for many important high-nitrogen compounds are often unknown or determined with relatively large uncertainties. Today quantum chemical calculations can be used successfully for prediction of thermochemical properties or analyzing of experimental data. The Gaussian-n family methods (G4 and G4(MP2)) combined with atomization reaction were tested in their possibilities to quantitatively estimate the values of enthalpy of formation. To get the accurate gas-phase enthalpies of formation, the quantum chemical calculations combined with isodesmic reaction scheme were used in this study. A set of internally consistent values of enthalpies of formation of nitrogen-containing compounds has been obtained. Among these are nitro compounds, nitramines, amines, heterocycles, and azides with different architecture and functional groups. In addition the reliable values of sublimation enthalpy were used to parameterize the Politzer equation for computing the heat of sublimation of high-nitrogen compounds.

Synthesis, characterization and mechanical properties of polyether polyurethane azide elastomers

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Keywords: mechanical properties; polyether polyurethane azide elastomers; melt-cast explosive.

A new energetic polymer used for melt cast explosives, polyether polyurethane azide elastomer using prepolymerized glycidyl azide polymer (GAP) as soft segments, polyurethane being prepared with 2,6-dinitro-1,4-diphemethyol and 4,4'-diphenylmethane diisocyanate (MDI) as hard segments, was synthesized starting from 2,6-dinitro-1,4-diphemethyol, epichlorohydrin and MDI via a three-step process involving initial etherification, subsequent azidation of polyether and then crosslinking. Polyether polyurethane azide elastomer was characterized by Gel permeation in chromatography (GPC), Fourier transform infrared spectrum(FT-IR), and 1H techniques. By controlling the proper reaction conditions, polyether polyurethane azide elastomers could be prepared with number average molecular weight (Mn) in the range of 8.68×103 1.56×104 and polydispersity index (Mn/Mw) in the range of 1.3 1.73. Moreover, mechanical properties of polyether polyurethane azide elastomers were measured through compressive test, comparing compressive strength and compressive deformation with that of RDX-based melt cast explosive. The experimental results showed the compressive loading,compress strength and compress deformation of melt cast explosive with 1.0% polyether polyurethane azide elastomers increased by 7.1%,9.8%,22.5% , indicating a good additive to increase the mechanical property of melt cast explosives.

Controlling a polymorphic transition in 2,4-dinitroanisole using crystal doping

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Keywords: 2,4-dinitroanisole; polymorphism; crystal doping; solid solution; polymorph transition suppression.

Irreversible thermal expansion of DNAN up to 15% has been previously observed when samples are temperature cycled between 219 K and 344 K (-54 oC to +71 oC), however only 1% is considered acceptable. Six polymorphs of DNAN have currently been identified under a range of temperatures and pressures. One important transi-tion occurs at 266 K. The polymorphic transition from DNAN-II to DNAN-III is a sub-tle phase transition involving ordering of the disordered nitro groups and a jump in the monoclinic β-angle. This transition may be responsible for the irreversible growth experienced by DNAN. Doping of DNAN using 5% 2,4-dinitrotoluene has been shown to suppress the II-III transition to below 240 K. The effect of increasing the dopant to 10% causes further suppression to below 210 K and is therefore no longer within the temperature range where thermal expansion has been shown to be an issue. The polymorphic transition in the doped DNAN samples is broadened over a range of >20 K, in stark contrast to the abrupt transition observed in undoped DNAN. Comparable suppression was also observed by doping DNAN with 1,3-dinitrobenzene.

Thermal stability of p-dimethylaminophenylpentazole

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Keywords: pentazole; thermal stability; decomposition.

The thermal stability of p-dimethylaminophenylpentazole(1) in the solid phase has been thoroughly investigated. The decomposition process of 1 has been verified by a combination of differential scanning calorimetry (DSC), thin-layer chromatography (TLC), temperature-programmed FTIR, and Raman spectroscopy. FTIR and Raman spectra were also calculated to corroborate the results. It was found that 1 could be handled below 20 °C´ without any obvious deterioration, but it decomposed sharply at 56 ´°C. The calculated FTIR and Raman vibrational frequencies were in accord with the experimental values.

An improved method for the synthesis of 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diaza-isowurtzitane

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Keywords: chemical synthesis; mild conditions; energetic materials.

4,10-Dinitro-2,6,8,12-tetraoxa-4,10-diazaisowurtzitane, also known as TEX, is a state-of-the-art explo-sive, with properties that comply with the requirements of explo-sives used for military purposes. The present study shows an improved synthesis method of TEX, which could be applied both on laboratory and industrial scale. This energetic material may be considered for inclusion in insensitive munitions, taking into account that it is easy to fabricate, both from technical and economical points of view, it has a good processability (through melting, casting or pressing), and it pre-sents a low sensitivity against mechanical and electrical stimuli.

A theory study on the structure characteristics of explosive crystals and its effect on sensitivity against external stimuli

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Keywords: crystal structure; sensitivity.

The sensitivity differences can be caused by chemical components, polymorph, crystal faces and crystal quality, which make us conscious of that the packing character is another key to determine the sensitivity, besides molecular stability. Using theoretical means like geometry description, packing coefficients, QCAIM, Hirshfeld surface with 2D fingerprint plot and the supramolecular synthons, we studied the effect of the crystal packing structures on the sensitivity. For the monocomponent explosive, the distinct difference between the low-sensitivity high-energy explosives (LSHE) and the sensitive high-energy explosives (SHE) on the molecular structure and the packing of the crystal is that the LSHE is much more easily sliding. The intermolecular interaction changes less when sliding. And the possible reason for improving sensitivity by energetic cocrystallization is attributed to the higher stability of the component molecule added or improved crystal packing. We also studied the effect of twin crystal of HMX on the shock sensitivity with the method of ReaxFF reactive force field. The twinned HMX can make a remarkable rise of the shock sensitivity, consistent with the experimental results. The effect on the shock sensitivity of this kind of defects can be attributed to the increase of the free volume in the crystal, the hot spot formed in the place where the free volume increased. The study of crystal structure characteristic is advantageous to the multiscale design of explosives.

An improved electrical conductivity test method for detonation products

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Keywords: electrical conductivity method; detonation products; TNT.

An improved electrical conductivity measurement method for detonation products is presented, which is developed on the basis of the traditional coaxial measurement. Compared with the traditional coaxial measurement, there are three aspects which have been improved, the details are as follows: (1) the structure and material of the tube were optimized in order to reduce the tube deformation; (2) the tops of the center electrode and the copper tube are placed in the same plane, which will eliminate the effect of the bypass resistor. Meanwhile, to reduce the instability of detonation growth process, the testing explosive is detonated by shock wave; (3) the measurement circuit is also improved. The electrical conductivity of detonation products in TNT, which was measured by this method, is in reasonably good agreement with previous experimental data.

Inelastic neutron scattering phonon spectrum of FOX-7 from first principles calculations

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Keywords: 1,1-diamino-2,2-dinitroethene; first principles; molecular structure; inelastic neutron scattering spectrum; vibrational properties.

The molecular geometry and inelastic neutron scattering phonon spectrum and vibrational properties of isolated molecule and crystal of 1,1-diamino-2,2-dinitroethene are investigated with first-principles calculations. The structural results were found to be in good agreement with experimental X-ray diffraction data and previously reported calculations. The vibrational frequencies calculated from FOX-7 molecule agree well with literature. The geometry of crystalline molecule is close to the experiment result. The vibrational frequencies of FOX-7 molecule and crystal are compared and the result indicates that intermolecular hydrogen bond can affect vibrational mode differently and frequency shifting correlates with geometry of isolated molecule and solid-state molecule. The inelastic neutron scattering phonon spectrum are calculated for isolated molecule and crystal. There are multiple peak values below 2.5 terahertz for crystal, and the trend and values of the phonon spectrum are coincident with that from terahertz time-domain spectroscopy experiment which demonstrates the validity of first-principles calculations.

Microreactor flow synthesis of the secondary high explosive 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105)

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Keywords: secondary high explosives; microreactor; flow chemistry; LLM-105.

The secondary high explosive 2,6-diamino-3,5-dinitropyrazine-1-oxide, or LLM-105, has been synthesized using a commercially available flow microreactor system. Investigations focused on optimizing flow nitration conditions of the cost effective 2,6-diaminopyrazine-1-oxide (DAPO) in order to test the feasibility and viability of flow nitration as a means for the continuous synthesis of LLM-105. The typical benefits of microreactor flow synthesis including safety, tight temperature control, decreased reaction time, and improved product purity all appear to be highly relevant in the synthesis of LLM-105. However, the process does not provide any gains in yield, as the typical 50-60% yields are equivalent to the batch process. A key factor in producing pure LLM-105 lies in the ability to eliminate any acid inclusions in the final crystalline material through both a controlled quench and re-crystallization. The optimized flow nitration conditions, multi-gram scale up results, anal-yses of sample purity, and quenching conditions for purity and crystal morphology control will be reported.

Study of decomposition kinetics of binder system based on HTPB using different techniques and methods

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Keywords: HTPB; thermal decomposition; model-free method; model fitting.

Thermal behavior and decomposition kinetics of a binder system based on hydroxyl terminated polybutadiene (HTPB) were studied by using different techniques. Vacuum stability test (VST) STABIL and Thermogravimetric analysis (TGA/DTG) techniques were used. Isothermal and non-isothermal methods were applied to determine the decomposition kinetics. The kinetic triplet parameters were determined by using Model-fitting methods. Model-free (isoconversional) method was applied to calculate the activation energy of the binder system. From TGA/DTG measurements, it was concluded that the decomposition process of HTPB binder system has two steps. While only one step decomposition was observed using VST. The calculated activation energy, obtained by using Kissinger method, Ozawa,Flynn and Wall (OFW) method or Kissinger-Akahira-Sunose (KAS) method, had a value of 208-212 kJ/mol. The VST was also used to obtain approximate value of the activation energy.

Nitration of 3,6-Bis(aminoazole)-1,2,4,5-tetrazine derivatives - towards more oxygen-balanced nitrogen-rich energetic materials

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Keywords: nitrogen-rich compounds; synthesis.

One of the successful strategies for the design of promising new energetic materials is incorporation of both fuel and oxidizer moieties into the same molecule. Therefore, during recent years, synthesis of various nitro-azole derivatives, as compounds with more balanced oxygen content, became very popular. In the frame of this effort, we studied nitration of N3,N6-bis(1H-tetrazol-5-yl)-1,2,4,5-tetrazine-3,6-diamine 1 (BTATz) and its alkylated derivative N3,N6-bis(2-methyl-2H-tetrazol-5-yl)-1,2,4,5-tetrazine-3,6-diamine 2 using 15N-labeled nitration agent and analyzing products of these reactions by 15N NMR. It was shown that the nitration of both compounds takes place only on the exocyclic ("bridging") secondary amine groups. Possible tetranitro derivative N,N'-(1,2,4,5-tetrazine-3,6-diyl)bis(N-(nitro-1H-tetrazol-5-yl)-nitramide), with calculated Oxygen Balance of 0%, could not be observed in the reaction mixtures, even during the in situ monitoring. Following a similar strategy, new analog of BTATz – N3,N6-Bis(1H-1,2,4-triazol-5-yl)-1,2,4,5-tetrazine-3,6-diamine 3 was obtained and its nitration was studied. The reaction of compound 3 with HNO3-Ac2O nitration mixture resulted in formation of a new N3,N6-bis(3-nitro-1H-1,2,4-triazol-5-yl)-1,2,4,5-tetrazine-3,6-diamine derivative 4 in a moderate yield. Structures and properties of new compounds 3 (in a form of its perchlorate salt) and 4 were established by FTIR, NMR, MS, DSC, bomb calorimetry and x-ray crystallography. Important to note that compound 4 exhibits exothermic decomposition at 309°C (DSC), making it highly-promising insensitive energetic material for further development.

Synthesis and some physicochemical properties of 3-azido-4-(tetrazol-5-yl)-furazan

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Keywords: azidofurazan; nitrofurazan; 1,2,5-oxadiazole; tetrazole; amidrazone.

Synthetic routs for a new energetic compound – 3-azido-4-(tetrazol-5-yl)-furazan preparation are presented. The titled compound was prepared by four stages syn-thesis from amidoxime of 4-aminofurazan-3-carboxylic as a starting material. Condensation of this compound with triethylortoformate gives 3-amino-4-(1,2,4-oxadiazole-3-yl)furazan which was oxidized by hydrogen peroxide in sulfuric acid to 3-nitro-4-(1,2,4-oxadiazole-3-yl)furazan. The substitution of nitro group to hy-drazine one in the latter compound by the action of hydrazine is accompanied by reductive 1,2,4-oxadiazole ring opening and results in amidrazone of 4-hydrazinofurazan-3-carboxylic acid formation. Its diazotization in acetic acid by two moles of sodium nitrite gives 3-azido-4-(tetrazol-5-yl)-furazan.

Two-point initiation by plastic explosive channels

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Keywords: two-point initiation; detonation wave; plastic explosive.

A simple and inexpensive model for parallel and simultaneous two-point initiation was developed. A key component of the model is a cylindrical attenuator with two narrow channels filled with plastic explosive, which transforms one quasi-spherical detonation wave into two waves. This quasi-spherical wave was achieved with a simple combination of a detonation cap and a booster charge. The shape of the resulting detonation wave was experimentally determined in an acceptor cast explosive at different distances from the initiation line, which confirmed that a simultaneous initiation was achieved.

Reaction of S,S'-dimethyl-N-nitroimidodithiocarbonate with alkalis

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Keywords: S,S'-dimethyl-N-nitroimidodithiocarbonate; nitrimines; S-methyl-N-nitrothiocarbamate.

Reaction of alkaline hydrolysis of S,S'-dimethyl-N-nitroimidodithiocarbonate has been investigated. The product of complete hydrolysis of compound in aqueous medium is a sodium or potassium carbonate. Carrying out the reaction under controlled conditions allows to obtain a product of a nucleophilic substitution of one methylthio group – salts of S-methyl-N-nitrothiocarbamate. Potassium, sodium, ammonium and hydrazinium salts, as well as free S-methyl-N-nitrothiocarbamate were synthesized and characterized. Carrying out the hydrolysis reaction in ethanol leads to the formation of salts of ethyl-N-nitrocarbamate (nitrourethane). S-methyl-N-nitrothiocarbamate contains methylthio group, which can easily be replaced by the action of nucleophilic agents. This makes it possible to synthesize an energetic compounds containing nitrocarbamic group (–CO-NHNO2).

X-ray structure of methylenedinitramine

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Keywords: methylendinitramine; primary nitramines; X-ray analysis.

Methylenedinitramine (MEDINA)is well-known powerful explosive with a zero oxygen balance. Lattice parameters of MEDINA were determined from X-ray powder diffraction data over half a century ago. However, until today its structure has not been published in the literature. Given communication is devoted to molecular structure of MEDINA established by methods of X-ray analysis.

New pentaerythritol based energetic materials related to PETN

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Keywords: pentaerythritol tetranitrocarbamate; tetraammonium salt; physicochemical properties; detonation properties; exploding action.

A three step synthesis of a new pentaerythritol based energetic material was carried out. At the first step pentaerythritol tetracarbamate was obtained from pentaerythritol. At the second step the energetic material pentaerythritol tetranitrocarbamate was obtained. This material is thermally more stable and shows a lower sensitivity against friction and impact compared to the well-known pentaerythritol tetranitrate (PETN). At the third step the new stable explosive tetraammonium salt was obtained. A lot of physicochemical and detonation properties were studied for pentaerythritol tetranitrocarbamate and its explosive tetraammonium salt. The methods of X-ray diffraction, nuclear magnetic resonance, mass spectrometry, infrared spectroscopy, differential scanning calorimetry and sensitivity to different factors were used for that . Calculated results on the determination of exploding action of both energetic materials upon metal barriers were obtained in various statements. Gaussian 09, EXPLO5 V.6.02, Cheetah 2.0 and ANSYS 15.0 Autodyn computer programs were used for the calculations.

The analysis of explosive charge density and scaled distance influence on shockwave overpressure using response surface methodology

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Keywords: shockwave overpressure; RSM; Cyclotol 50/50.

This paper analyses the influence of explosive charge density and scaled distance on shockwave overpressure for cyclotol 50/50 using response surface methodology (RSM). Experimental data were obtained by measuring the shockwave overpressure at different distances for 0.4 kg explosive charge weight. Explosive charge density was varied as well. Shockwave overpressure was measured using piezoelectric probes set at different distances. RSM method is used to investigate and optimize the influence of dependent variables on shockwave parameters. Based on statistical analysis, the cubic model proved to be highly significant with very low probability values (<0.0001).The predicted model was successfully fitted with the experimental results giving COD greater than 0.99.

FOX-7-based melt-cast compositions – preparation and some properties

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Keywords: FOX-7; low-sensitive explosives; melt-cast explosive.

1,1-Diamino-2,2-dinitroethene also known as DADNE or FOX-7 is commonly expected to be a promising explosive combining comparatively high performance and low sensitivity. FOX-7 has appeared to be very useful for low sensitive formulations. A brief review of FOX-7-based compositions and their properties is presented in this paper. Moreover, melt-cast compositions based on FOX-7 were prepared on a laboratory scale and their properties were investigated. Sensitivity to impact and friction were determined, thermal stability and ignition temperature were established. The viscosity of compositions was measured. Some of detonation parameters were determined. The initial studies indicate FOX-7 -based formulations as a potential replacement of TNT in munitions.

Synthesis and studies of carbo- and heterocyclic compounds derived from the products of functionalization of 2,4,6-trinitrotoluene

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Keywords: 2,4,6-trinitrotoluene; functionalization; synthesis; properties.

Basing on the developed industrial techniques of utilization of 2,4,6-trinitrotoluene, some new approaches of its functionalization are presented. The synthesis of new carbo- and heterocyclic compounds and their activity in the reactions od bromination, azo-coupling, and O-acylation are discussed.

Research on detonation characteristics of nitrocellulose based propellants

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Keywords: detonation; detonation velocity; propellant; nitrocellulose.

Detonation characteristics of single and double based propellants were investigated. There were considered domestic propellants with different composition and grain dimensions. Detonation velocity was determined experimentally for cylindrical explosive charges with different initial density and diameter. The results were analyzed and compared with corresponding literature and calculated values.

Modeling of loss factors of elastomer binders of high explosive charges and composite rocket propellants to separate binder fractions with different molecular mobility used to follow aging

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Keywords: dynamic mechanical analysis; glass-rubber transition; modelling of loss factor; exponentially modified Gauss distribution; separation of binder fractions with different mobility.

The glass-rubber transition temperature of elastomer bonded composite rocket propellants and high explosives is an important property determining their in-service application. It is defined as the main maximum of the loss factor tand, which is determined as function of temperature by DMA (dynamical mechanical analysis) measurements at some forced sinu-soidal deformation at lower frequencies in the range of 0.01 to 100 Hz. With the term tran-sition the center part of the molecular rearrangement process is meant, in which the tran-sition from the energy elastic ('glassy elastic') to the entropy elastic ('rubbery elastic') behaviour, or vice versa, occurs. The loss factor of an elastomer binder is influenced by sev-eral factors: (1) filler type and content, (2) plasticizer type and content, (3) sterical hin-drance, (4) interaction forces between all ingredients, (5) polymer chain conformation of the elastomer, (6) curing type and agent. Because the loss factor region of most elastomers filled with rigid particles consists of several sub-transitions, which can change differently during ageing and deformation rate loading, a special modelling of the loss factor curve is presented using so-named exponentially modified Gauss distributions. Therewith a separation and a quantification of the molecular rearrangement regions or binder mobility frac-tions is achieved, after the application of a suitable baseline correction function to the loss factor curve.

Effect of the ignition procedure on the temperature sensitivity of the combustion rate of gun propellant

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Keywords: closed vessel tests; ignition condition; firing temperature; gun propellant; deterrent; propellant combustion rate.

The temperature sensitivity of the combustion rate of a spherical deterred propellant has been established using closed vessel tests. The effect of ignition procedure on the temperature sensitivity of combustion rate has been determined. Different ignition mixtures of oxygen and methane have been investigated. These ignition systems are compared with the commonly used ignition by black powder. It has been observed that the temperature sensitivity of the combustion rate can be related to the homogeneity of the ignition of the propellant.

Description of explosion-like reactions in halovinyl polymers on impact

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Keywords: sensitivity to impact; halovinyl polymers.

In experiments on impact on drop-weight machine us earlier unknown phenomenon explosion-like reactions in thin-layer pressed (0,3-0,5 GPa) samples haloidvinyl polymers - polyvinylchloride (PVC), polyvinylydenftoride (PVDF) and so forth is revealed. These reactions initiated by impacts with energy more 10 J and impact pressure more 1 GPa, are shown in the form of the sound effects which intensity several times exceeds a sound of the idling (not equipped) impact, caustic smoke and, in rare instances, light flashes. However such conclusion is precipitate, as investigated polymers do not possess detonation ability and are not inclined to support of self-propagating explosion processes. From Theory HE it is known that the major factors defining explosion character of chemical transformation of substance, and also its destroying action, are exothermicity, gas evolution and high velocity of passing these processes. The analysis finding by wire strain gage records of impact pressure shows that explosion-like reactions in polymers proceeds during time of strengthening failure (brittle fracture) of samples, i.e. during small interval of time 10 ms, this process testifying to high velocity of explosion-like reactions. It is known also, that considered polymers thermally unstable and at the heating they decompose mainly on solid polyene and carbon structures and gaseous halogen hydride - NSl, HF. The last, being formed at high (0,5 GPa) impact pressure, with the high velocity (0,1 km/s) expire from a narrow backlash between the striker and an anvil, creating in surrounding air atmosphere characteristic sound effect of explosion. The considered experimental facts testify that explosion-like processes observed at failure of polymeric samples, have much in common with the phenomenon of initiation of explosion at impact on charges solid HE and consequently the description of their course is obviously possible for drawing by analogy to the available workings out used for an explanation of mechanical initiation of solid explosives. Among all polymers physical-chemical and mechanical characteristics of PVC are most studied and presented in numerous works. Therefore further we will describe a picture of initiation of polymers at impact on the PVC example though all conclusions of the work will concern to all specimens of thermally unstable polymers.

Research of the test method of volume expansion coefficient for typical explosive

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Keywords: pressed explosive; volume expansion coefficient; liquid immerging method.

The volume expansion coefficient of typical pressed explosive was tested by the method of liquid infiltration,which was a method chalked up the volume expansion coefficient by immerging the sample in appropriate liquid and testing the changing of volume of the liquid and sample. Compatibility test and equilibrium swelling method were used for the confirming of the suitable liquid for typical sample,such as pressed explosive A. As results of theoretical calculation in a wide temperature range and screening expriment, the appropriate size of typical sample was height of 20 mm and 19 mm in diameter in the sample chamber, the size of which was height of 21.15 mm and 19.95 mm in diameter.

Salts of 4-picryl-3,5-dinitropyrazoles with high decomposition temperatures

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Keywords: high temperature explosives; synthesis; charaterisation.

As the boreholes of oil wells are getting deeper and deeper, the need for explosives with high decomposition temperatures increases. One very promising family is salts of 4-picryl-3,5-dinitropyrazole, whose synthesis hitherto has not been described.

The starting material of the synthesis is TNT, whose transformation into more valuable compounds has been studied extensively. This well-known compound was subjected to a double Vielsmeier-Haack reaction. The obtained product was hydrolysed into a dialdehyde. Cyclisation of this compound with hydrazine hydrochloride resulted in 4-picrylpyrazole and subsequent nitration provided 4-picryl-3,5-dinitropyrazole.

The potassium and calcium salts of this compound were prepared and characterized. They both have very high decomposition temperatures, especially so the latter, whose onset in the DSC occurred at 385 °C. This is superior to HNS, whose decomposition temperature is 316 °C under the same conditions.

Advanced kinetic analysis for life-time prediction of energetic materials

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Keywords: safe storage life prediction; kinetic parameters; AKTS Thermokinetics software.

Abstract: In the present study, we propose the safe storage life prediction of propellants in different temperature mode via AKTS Thermokinetics software by means of computation of reaction kinetics, which was evaluated from the dates of stabilizer content under thermal accelerated aging at temperature of 95, 90, 85, 75 and 60°C. The kinetic parameters are calculated using the truncated Sestâk-Berggren (SB) [1]approach and further verified by using the Akaike and Bayesian information criteria[]. In order to demonstrate this prediction, the estimation under depot atmospheric temperature mode has been compared with the real experimental results. Presented results indicate that the date of stabilizer depletion (6.6%) of the 24-year-storage propellant is approximately close to that of estimation (6.7%). Presented results indicated that the life-time of propellants can be predicted with great accuracy.

Shock response of large aggregate concrete

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Keywords: shock; concrete; blast; Hugoniot.

A series of plate-impact experiments were conducted using the large bore single stage light gas gun at Imperial College London to characterise the shock response of a large aggregate concrete. A reverberation plate-impact technique employing an array of optical velocimetry probe was used to measure Hugoniot data and subsequent release states for peak stresses in the range 2-13 GPa. The use of multiple velocimetry probes enabled quantification of the local fluctuations in particle velocity arising from the heterogeneous nature of the large aggregate concrete being investigated. Additionally, Hugoniot data was also measured using small-scale explosive loading experiments, demonstrating the feasibility of such an approach. The measured data are compared with results from previous studies.

An environmental friendly method for the preparation of 5-nitrotetrazole sodium salt

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Keywords: Sandmeyer reaction; green chemistry; safety scaling; 5-nitrotetrazole sodium salt; adsorption; active carbon; chromatographic purification.

The report is devoted to the development of a method for laboratory-scale synthesis and purification of 5-nitrotetrazole sodium salt which is the key precursor for various energetic materials. The proposed method meets the requirements of ecological safety and relates to the so-called “green chemistry” technologies. The proposed method is suitable for safety scaling. Keywords: Sandmeyer reaction, ”green” chemistry, safety scaling, 5-nitrotetrazole sodium salt, adsorption, active carbon, chromatographic purification

Energetic derivatives of 5-(5-amino-2H-1,2,3-triazol-4-yl)-1H-tetrazole

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Keywords: energetic materials; primary explosives; secondary explosives; heterocycles; X-ray structures.

This study presents the preparation of the novel compound 1-(4-amino-2H-1,2,3-triazol-5-yl)tetrazole and its further derivatization, including azido, nitro, diazonium and diazene groups. The ability of salt formation is demonstrated with both nitrogen-rich and metal cations. The energetic compounds were comprehensively characterized by various means, including vibrational (IR, Raman) and multinuclear (1H, 13C, 14N, 15N) NMR spectroscopy, mass spectrometry, DSC and single-crystal X-ray diffraction. The sensitivities towards selected outer stimuli (impact, friction) were determined according to BAM standards.

Quantum chemical modeling of the enthalpy of formation and acidity of polynitroazole salts

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Keywords: heat of formation; heat of salt formation; acid dissociation; polynitroazoles; ammonium salts; DFT; CBS; VBT.

The thermochemical characteristics and acidity of polynitroazole ammonium salts were investigated. The Glasser-Jenkins method was modified, which significantly improved the accuracy of calculations of formation enthalpies. The acidity of a few polynitroazoles in water was computed and a lack of correlation between their acidity and the enthalpy of salt formation was revealed.

Synthesis and crystallization of HNF(Hydrazinium Nitroformate) as an eco-friendly oxidizer

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Keywords: oxidizer; nitroform; synthesis; crystallization.

The explosion of traditional explosives and propellants is a big environmental issue. Es-pecially, ammonium perchlorate (AP) which is commonly used as an oxidizer in various energetic materials generates a large amount of HCl gas and atmospheric pollutants. Among the several oxidizers, hydrazinium nitroformate (HNF) is a good candidate to re-place ammonium perchlorate (AP) because it has high density, pressure index and also generates less pollutants and less smog. There are many methods reported to synthesize HNF from isopropyl alcohol (IPA) or acetic anhydride (AA) used as starting materials. In this study, more than 98% pure HNF was synthesized and we measured the solubility in some alcohol solvents at different temperature from 283.15K to 323.15K according to the isothermal method. And then, HNF crystals were obtained from crystallization process.

Synthesis and investigation of energetic transition metal complexes using di(1H-tetrazol-5-yl)methane as nitrogen-rich ligand

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Keywords: primary explosives; energetic coordination compound; tetrazole.

The synthesis of di(1H-tetrazol-5-yl)methane (1, 5-DTM), starting from commercially available sodium azide and malononitrile, is described. This tetrazole was fully characterized and investigated for use as a nitrogen-rich ligand in various energetic transition metal complexes. Obtained coordination compounds were characterized using single crystal X-ray diffraction, IR spectrometry, elemental analysis and differential thermal analysis (DTA). The sensitivities to external stimuli (impact, friction and electrostatic discharge) were determined according to Bundesamt für Materialforschung (BAM) standard methods.

Numerical simulations of initiating strength of detonators

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Keywords: TKX-50; MAD-X1; underwater test; Autodyn.

Currently, numerous different detonators are commercially used e.g. electric, non-electric, and electronic. Most of them contain pentaerythritol tetranitrate (PETN) as a secondary explosive. During the action of the detonator a sufficiently strong impulse has to be obtained in order to ignite the secondary explosive (an acceptor charge). According to recommendations of the European Committee (Council Directive 93/15/EEC) the determination of the initiating capability of detonators is determined using an underwater test [EN 13763-15, Determination of equivalent initiating capability]. This work focuses on the estimation of the initiating strength of detonators containing as a secondary explosive either TKX-50 (dihydroxylammonium 5,5'-bis(tetrazolate-1N-oxide) or MAD-X1 (dihydroxylammonium 5,5'-bis(3-nitro-1,2,4-triazolate-1N-oxide) and comparison of them with currently used explosives. Detonation parameters (heat of detonation, detonation temperature, detonation pressure, and detonation velocity), Jones-Wilkins-Lee isentrope, and the energy of detonation were computed using the EXPLO5 V.6.01 program. Numerical modelling of the action of detonators were carried out using the ANSYS AUTODYN software. A geometrical model of the water tank, the location of the detonator, and a gauge point used as pressure sensor were used according to the European Standard. Analogous results were also obtained for other explosives such as PETN, RDX, and HMX. A detailed description of numerical modelling is presented.

Termochemistry of salts of 5,5'-azotetrazole with nitrogenous bases

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Keywords: salt of 5,5'-azotetrazole; calorimetry; enthalpy of formation.

Salts of 5,5'-azotetrazole (AzT) with organic bases are considered as perspective components for gun powders, gas-generating compositions and "green" double-base and composite propellants. However, existing data on the enthalpies of formation is most contradictory and knotty. The aim of the present work was to obtain more accurate information on the enthalpies of formation of a series of salts of 5,5'-azotetrazole with onium bases. The calorimetric measurements were carried out in a bomb calorimeter with a modified oxygen bomb. Samples to test were burnt in free the pending state, without using a crucible. The enthalpies of formation were calculated from measured heats of combustion.

Energy properties and thermal decomposition kinetics of triazine derivatives

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Keywords: high energy compounds; thermal decomposition; kinetics; triazines; enthalpy of formation.

A trinitromethyl group is specific of a high oxygen balance and therefore it is of considerable interest as a fragment of high energy molecules. Researches on the synthetic pathways for trinitromethyl derivatives of heterocyclic compounds are growing in number each year. However the publications, as a rule, do not communicate experimental data on the enthalpy of formation and thermal stability. This paper discusses the thermomechanical and kinetic properties of a few 1,3,5-triazines that incorporate trinitromethyl and azide substituents. Syntheses and measurements of combustion energies were performed until a complete convergence of combustion energies within a few batches of specimens. Calorimetric measurements of combustion energies were done using a precision automatic calorimeter of combustion with an isothermal jacket. The kinetics of liquid phase thermal decomposition of 1,3,5-triazines in the isothermal conditions was studied by a manometric method. Gaseous decomposition products were identified by mass spectrometry in combination with a fractional condensation method. The kinetics of thermal decomposition of 2,4-diazido-6-trinitromethyl-1,3,5-triazine and its derivatives was described by a first order equation. Rate constants, activation energies and pre-exponential reaction factors were determined. Dissociation energies of the C – NO2 bond were found. The composition of gaseous products of thermal decomposition was defined. IR spectra of the reagents and their decomposition products were reviewed. A decay of the trinitromethyl group appeared a limiting reaction step. Thermal decomposition in the non-isothermal conditions proceeded by two macroscopic stages and of note is that the trinitromethyl group decomposed in the first stage. Aggregate stoichiometric equations for the reactions were derived.

Electromagnetic method in determination the detonation parameters of ammonium nitrate explosives

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Keywords: electromagnetic method; ammonium nitrate based mixtures; mass velocity.

This paper presents the results of the study detonation parameters for minced and porous ammonium nitrate (AN) with different amount of inerts such as sodium chloride and silica. Using electromagnetic method the shape of detonation waves in explosive mixtures were determined. For selected ammonium nitrate based mixtures detonation parameters such as detonation velocity, mass velocity and reaction time behind the detonation wave front were measured.Additionally, one of the experimental result was confirmed in numerical simulations.

Tubing side cutter – simulation and performance testing in borehole

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Keywords: linear shape charge; removing breakdown; restoring circulation in borehole.

The research team have developed a new instrumentation equipment, remedying loss of circulation in borehole. The project used institutes experience in scope of designing, construction optimization and production of linear shaped charges, intended for cutting steel sheets, pipes and structures. A part of works, connected with tubing side cutter designing and optimization was shown. Furthermore a part of optimization research – simulation computer testing with Ansys Autodyn2D software of tubing side cutter functioning in borehole was presented. The developed tubing side cutter (for 2 3/8" tubing) ŁKN-150-60-34/150 type, i.e. 34 mm OD was subjected to fire ground tests and performance testing.

Kinetics and mechanism of the thermal decomposition of 2,4-dinitro-2,4-diaza-6-R-6,6-dinitrohexane

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Keywords: kinetics; steric constants; correlation; reaction center.

Kinetics and mechanism of the thermal decomposition of gem-dinitroethyl-di-N-nitramines is investigated. The limiting stage is established and its activation parameters are determined. It is shown that logarithms of the rate constants and activation energies correlate with the steric constants of substituents Es. The received correlation equations allow forecasting synthesis of unstudied compounds of this row with the set parameters for chemical stability.

Characterization of tetraamminecopper salts

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Keywords: complex salt; copper; explosives; enthalpy of formation; explo5.

This paper deals with basic characterization of the complex salts tetraamminecopper nitrate (TACN) and tetraamminecopper perchlorate (TACP). The salts were prepared via the reaction of the corresponding simple copper salts with ammonia in an aqueous solution. The composition of the products was determined using elemental analysis and infrared spectrometry. Combustion calorimetry was used for determination of the enthalpy of formation and the density was determined by pycnometry. Detonation parameters were then calculated using the Explo5 thermochemical code.

Evaluation of the effect of plasticizers on the DMA loss factor, the thermal and mechanical properties of Desmophen 2200 based elastomers used for composite propellants

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Keywords: energetic plasticizer; Desmophen D2200; DMA measurements; loss factor modelling; glass-rubber transition.

The aim of this work was to evaluate the effect of changing the plasticizer type and its amount on the DMA loss factor curve, glass-to-rubber transition temperatures and mechanical properties of Desmophen® 2200 based binders. One of the main challenges concerning energetic materials regards the establishments and evalua-tions of new binders as alternative for the HTPB based composite rocket propellant formulations currently on use on the western countries. For that reason not only new energetic binders are considered (e.g the polyether Glycidyl Azide Polymer, GAP), but also new energetic components such as energetic plasticizers, which consist of low molecular weight energetic polymers. Despite being inert, the polyester polyol Desmophen® 2200 (D2200®) has been investigated because of its good glass-to-rubber transition properties when mixed with polar energetic plasticizers. Also previous work has indicated that composite propellant based on D2200® binder mixed with 35% TMETN as energetic plasticizer can give good ballistic performance properties compared to HTPB and GAP based formulations. But the strain capability and glass-to-rubber transition are still an issue. Thus, in the present work different pure binder were formulated and characterized. The inert polar binder D2200® was mixed individually with TMETN, Bu-NENA, BDNPF-A, GAP-A, EGBAA and TEGDA in amounts of 5, 20 and 35%, and cured with Desmodur® N3400. The cured elastomers were characterized using torsion DMA, tensile properties and thermal properties. The loss factor curves obtained by DMA were modelled with exponentially modified Gaussian (EMG) functions, and the effects of the plasticizer on the EMG parameters were evaluated. The description of the shift of the glass-to-rubber transition temperature with plasticizer concentration is undertaken.

Thermal stability determination at almost full filling of the reaction volume

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Keywords: gas release; mesurement.

When one has to determinate the thermal stability of energetic materials it is very important that the degree of filling the sample under investigation in the reaction volume (m/V , where m- the sample mass, V-all storage vessel volume), where gaseous decomposition products are stored, would adequate to the values of m/V at which the real energetic material would be really stored. Otherwise the thermal stability forecast will be wrong. The investigation is devoted to developing a method of determining the depth of the decomposition of energetic materials and compositions at temperature 20-80° C at m/V values close to the density of the material under investigation. Test procedure of polymerized composites as well as individual compounds or their mixtures has been developed. The procedure allows to determine the amount of gaseous decomposition products such as nitrogen, hydrogen, carbon monoxide, carbon dioxide, nitrous oxide, nitrogen monoxide) during the exposure at the predetermined temperature and time

Heat-resistant energetic materials of polynitroaromatic substituted difurazano[3,4-b:3',4'-e]pyrazine

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Keywords: energetic materials; heat-resistant; difurazano[3,4-b:3',4'-e]pyrazine; crystal structure; properties.

The synthesis of polynitroaromatic substituted difurazano[3,4-b:3',4'-e]pyrazines was described. The structure of 4,8-di(2,4-dinitrophenyl)difurazano[3,4-b:3',4'-e]pyrazine (DDNPDFP) was confirmed by single-crystal X-ray. All products were determined by 1H NMR, 13C NMR and IR spectroscopy, elemental analysis as well as differential scanning calorimetry. These compounds showed good thermal stability with exothermic decomposition peaks in the range of 283°C to 415°C. Impact sensitivity and calculated explosive performances were also reported for these energetic materials. All result suggested that polynitroaromatic substituted difurazano[3,4-b:3',4'-e]pyrazines have the potential to be useful heat-resistant explosive materials.

Preparation and testing of thermobaric composites

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Keywords: TBX; composite explosives; slurry method; wet method; aluminium combustion.

Thermobaric explosives (TBXs) are a new type of high destructive weapons. These fuel-enriched heterogeneous explosives overcome ideal high explosives shortcomings by the generation of a long-lasting traveling pressure wave and significant high thermal effects. They are extremely effective and destructive in enclosed spaces due to their ability to produce a high level of quasi-static pressure (QSP). This paper reviews current status of thermobaric explosives with a special attention to composite thermobarics and layered charges. Also, a new safe, low cost and non polluting method for obtaining composite thermobaric granular formulations is described. Each macroscopic granule obtained by this method is being itself a complete multi-components energetic composition, homogeneous or with a core-shell structure. The quality of granules and the core-shell structure have been verified by Optical Microscopy and Scanning Electron Microscopy (SEM). Several thermobaric composites with different compositions have been formulated using this method. Impact and friction sensitivity have been determined. Quasi static pressure from homogeneous and layered charges made from each composition has been measured in 150 dm3 explosion chamber and compared to the theoretical ones calculated using a thermochemical code. Finally, important conclusions are drawn.

Intermolecular interaction of mononitrotoluene plasticizers with TNT and RDX: an experimental and computational study

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Keywords: quantum-chemical method (QM); molecular dynamics (MD); nitroaromatic plasticizer; intermolecular interaction; TNT; RDX.

Intermolecular interaction of nitroaromatic plasticizer (mononitrotoluene) with TNT and RDX was experimentally and theoretically investigated. The basis set superposition error (BSSE) and interaction energy of TNT, RDX and plasticizers were computed at MP2/6-311++G** levels. Compared with the weak Einter between RDX and TNT (−1.586 kJ/mol), Einter between the o-nitrotoluene and TNT and RDX can increase to −131.557 kJ/mol and −48.487 kJ/mol, indicating there is strong intermolecular-interaction. SEM imagines also show that mononitrotoluene could form layered deposits in TNT and closely surround RDX crystalline. MD simulation results indicate that tensile modulus of (100) TNT and (100) RDX increases when introducing mononitrotoluene plasticizers separately, which agree with the experimental phenomenon of the Brazilian disk test

Investigation of sodium azide influence on detonation parameters of aluminized explosives

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Keywords: explosive performance; aluminized explosives.

Explosive transformation of explosives containing sodium azide is examined. Sodium azide (NaN3, SA) is considered as the component enhancing nitrogen content in the explosive mixture. Aluminized mixtures with alumina in powdered (Alp) or flaked (Alf) forms were considered. The performance (NaN3, SA) explosives was enhanced by addition of hexogen (RDX). A comparison of explosive performance of mixtures in which sodium azide was replaced by ammonium nitrate (NH4NO3, AN) is made. Detonation and constant volume explosion parameters at experimentally proved densities are evaluated. The rise of nitrogen content introduced by addition of NaN3 results in formation of aluminium nitride AlN(s). This is accompanied by considerable rise of explosion energy. On contrary, decrease in amount of products in gaseous phase results in lowering of detonation velocity.

Some chemical properties of ferrocenylbutanedioles

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Keywords: ferrocene derivatives; vulcanization accelerators; modifiers of rubber; butanediol.

Successful use of ferrocene derivatives as vulcanization accelerators and modifiers of rubber products constantly demands all new substances with multiple reaction centers allows synthesis on their basis a wide range of different compounds. For this purpose, we carried out by reacting 1-ferrocenyl-1,3-butanediol and 1,1-di (1,3-hydroxybutane) ferrocenilene aniline under acidic catalysis. The studied reaction conditions and a method of separating substances perfected. The structure of the synthesized compounds was proved by IR, NMR spectroscopy and elemental analysis.

Fluctuation model of laser initiation of primary explosives

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Keywords: laser initiation; primary explosives.

Recently proposed a new fluctuation model of the explosion initiation of energetic materials with pulse action. This model is based on the idea of the statistical distribution of the centers of origin of the reaction of explosive decomposition of the sample volume. The model allows a unified explain the appearance of craters (cavities) on the surface of samples of secondary explosives under intense pulsed action, and the nature of the experimentally obtained dependence of the induction period and the level of initiation threshold for initiation of PETN. We hypothesized that for primary explosives, should taken into account the features: We believe that unlike secondary explosives to initiate primary explosives the creation of sufficient at least one reaction center, in the event that the reaction is distributed over the entire sample. This assumption is based on the previously obtained data on the topography of the glow accompanying the explosive decomposition of silver azide at a uniform laser excitation of the sample. So, the model has been redesigned and held its experimental verification. The object of investigation used whiskers silver azide with characteristic dimensions of 2000×100×100 mm^3. Initiation of the explosion was carried out by using YAG: Nd laser LDPL10M (1064 nm, 10 ns). Were experimentally obtained explosion probability curves of silver azide with simultaneous recording of the light emission signal. It is shown that the experimental results agree with calculations based on the proposed model for the initiation of the primary explosives. All of this allows us to estimate the possibility of the proposed model as a promising tool for the description of a number of laws pulse initiation primary explosives.

Minimum burning pressure of AN-based explosives determination using OZM research MBP Vessel

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Keywords: ammonium nitrate; safety; industrial explosives.

Ammonium nitrate based explosives (ANEx) are the most common of all energetic materials. Although are ANEx studied for many years, today there are still very serious accidents associated with thermal stress of these explosives at elevated pressure. Presented paper deals with dependence of unspecified heavy anfo sample decomposition under elevated pressure and defined thermal stress. Pressure dependence on heating time, points of interest of described dependence and basic construction of MBP Vessel are presented as well.

Thermal stability of plastic bonded explosive

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Keywords: thermal stability; PBX.

In this paper the thermal stability of Plastic Bonded Explosive (PBX) is presented. The experiments were limited to three following method: deferential thermal analysis (DTA), decomposition temperature in Wood's alloy and Slow Cook of Test (SCO). The samples of PBX were analysed in order to determine the sensitivity level to different thermal stimuli.

Attenuation of blast waves from detonation of binary mixtures of liquid oxidizer and solid fuel by mobile barriers

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Keywords: blast wave; shock in air; attenuation; binary mixture.

The ability of concrete mobile barriers to attenuate blast wave was tested on three types of barriers. The non-ideal explosive investigated in this paper was binary mixture of liquid oxidizer and solid fuel. The results indicate that the efficiency of mobile barriers in attenuating blast wave is very low and they would in reality work only as a fragment catching elements.

Computer simulation of thermal decomposition mechanisms for nitro-derivatives of 1,3,5-triazine

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Keywords: 1,3,5-triazine; 2,4,6-trinitro-1,3,5-triazine; 2,4,6-tris(trinitromethyl)-1,3,5-triazine; simulation of thermal decomposition.

On the basis of previously developed methodology for simulation of thermal decomposition mechanisms of organic compounds, computer modeling the thermolysis process of 1,3,5-triazine, 2,4,6-trinitro-1,3,5-triazine, and 2,4,6-tris(trinitromethyl)-1,3,5-triazine was performed. Further, in the framework of the density functional theory (DFT) on B3LYP/6-31G*, the activation energy of the reactions at the initial stage of decomposition process was calculated and screening the most favorable pathways of compounds decay was carried out. The results of computer simulation were compared with experimental data.

The experimental determination of high-safety electric blasting cap operation time

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Keywords: non-primary explosive high-safety blasting cap; operation time.

The determination method of non-primary explosive high-safety electric blasting cap (BC-I-HS, NTREM-2012, -2013, -2014) operation time was designed. It was shown that this method can be used both for the whole BC-I-HS operation time determination and for the determination of operation time of separate parts of BC-HS: electric match, metallic cylindrical confinement (MCC) with PETN charge. The operation time of the EV-Zh electric match is in range from 1,88 to 2,03 ms, MCC operation time is in range from 1,27 to 1,37 ms and the whole operation time of BC-I-HS is in range from 3,15 to 3,4 ms. The BC-I-HS operation time meets the requirements of the Russian State Standard GOST 9089-75.

Synthesis of TNBI copper complex

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Keywords: TNBI; explosives; copper complex compounds.

The aim of this work was to synthesis a new complex compound containing copper as a coordination centre and 4,4',5,5'-tetranitro-2,2'-biimidazole (TNBI) as a ligand. We decided to combine TNBI which is relatively insensitive in form of salt with copper because cupric oxide is known as catalyzing agent. New complex of TNBI, copper and ammonia was obtained in the reaction of copper chloride, ammonia and TNBI in water solution. The compound could be used in modern weapon systems as an energetic ingredient and modificator in composite rocket propellants or in special pyrotechnics. It should fulfill the following main characteristics: to catalyze reaction to get cooler products, to enhance burning rate and to reduce sensitivity to mechanical stimuli of propellants. Stoichiometry of the compounds is: C6H8N10O9Cu. Properties of the title complex were investigated with nuclear magnetic resonance methods, thermal analysis, elemental analysis and atomic absorption spectrometry. Sensitivity to impact and friction were determined also.

Nitrocarbazoles: studies on their electron accepting properties, enzymatic reactivity and cytotoxicity

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Keywords: carbazole; nitrocompounds; DNC; TNC; quanto-mechanical calculations; enzymatic reactions; bioreduction; bioremediation; P450 reductase; spectra; toxicity.

Carbazole derivatives, possessing NO2 groups, are widely used in different fields of industry. 1,3,6,8-Tetranitrocarbazole (TNC) found its application in millitary practice for the illuminating and firring material formulations. In this work, six nitro- carbazole compounds (NCs) were synthesized by different nitration methods. The product structures were confirmed by spectral methods. The electronic characteristics of NCs and their electron-accepting potency were assessed by quantum mechanical methods. The enzymatic reactivity of NCs towards single- and two-electron/hydride-transferring flavoenzymes was examined. It has been found that the enzymatic reduction of TNC, as one of the most reactive NCs, was accompanied by formation of its main reductive azoxy-type product [MW=646.41] as confirmed by LC-MS method. The cytotoxic effects of certain selected NCs were examined against mammalian cell lines applying primary mice splenocytes. The concentrations of NCs for 50 % cell survival (CL50) were defined to be equal to 75 microM (TNC), 88 microM (1,3,6-TriNC), 50 microM (3,6-DNC) and 150 microM (3-MNC). The cytotoxic effect of NCs was found to be in the range of nitroaromatic model compound 1,3-dinitrobenzene (CL50=100 microM) and markedly lower than that of TNT (CL50=10 microM) or tetryl (CL50 = 6 microM).

Accelerating rate calorimetry - decomposition of nitroesters

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Keywords: thermal decomposition; nitroesters; calorimetry; ARC.

The thermal decomposition of six niroesters (methylnitrate, ethylene glycol dinitrate, propylene glycol dinitrate, glycerine trinitrate, erythritol tetranitrate and pentaerytritol tetranitrate) was studied with using of accelerating rate calorimetry. The classic heat-wait-search mode was used, the decomposition of samples took place in adiabatic mode. Pressure and temperature profiles were measured. Various possibilities of evaluation of achieved results (T, p, dT/dt, dp/dt) are discussed. Thermal stability increases in order ETN < EGDN,NG < PGDN < PETN < MeN. One of the main benefits of ARC is, that it enables measurement of thermal decomposition of liquid samples.

Effect of curing agents and plasticizers on the loss factor curves of HTPB-binders quantified by modelling

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Keywords: HTPB; curing agents; plasticizers; DMA loss factor; EMG modelling.

The key molecular level characteristic of elastomeric binder systems of composite rocket propellants is the glass-to-rubber transition region, which is mainly defined by the molecular mobility of the components in the polymeric network during phase transition from energy to entropy elasticity with respect to temperature. This feature has a strong dependence on temperature and is detectable by dynamic mechanical analysis (DMA) whereby obtaining the loss factor (tanδ= loss module / storage module) curves. HTPB R45HT based binders with four different types of isocyanates (IPDI, HDI, E305 and HMDI), with and without the common plasticizer DOA, were analyzed using loss factor curves obtained by torsion DMA. Exponentially modified Gauss distribution functions (EMG) were used to model the effect of the isocyanates on the molecular mobility (MM) of the polymeric networks. Developments of loss factor curves w.r.t. temperature showed distinct differences in the intensity of loss factor curves with different isocyanates in the following order HDI>IPDI»HMDI>E305. A relationship between MM observed by loss factor curves with tensile test was developed to support effect of each isocyanates on the binder network. Additional series of HTPB R45HT+IPDI binders were formulated with four different plasticizers (DOA, DOS, DOZ and IDP) to make further analysis on the effect of plasticizer types. Loss factor curves with different plasticizers had showed not such pronounced differences compared with the differences with isocyanate types. Mainly, the four plasticizers showed the same level of intensity in loss factor curves and maximum peak temperature Tg, except IDP, which provided with the lowest glass-to-rubber transition. Molecules, which can give more free volume to polymeric network due to fewer hindrances, in other words which restrict less the mobility of HTPB binder molecules. at low temperatures give the lowest Tg as in the case of IDP with R45HT+IPDI binder networks.

Enhancing the energetic properties of 5-(4-amino-1,2,4-triazol-3-on-5-yl)tetrazole by N-oxidation

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Keywords: triazolone; tetrazole; N-oxide; crystal structure; nitrogen-rich.

In our recent efforts to synthesize new high energetic materials which are based on nitrogen-rich heterocyclic systems, 5-(4-amino-1,2,4-triazol-3-on-5-yl)tetrazole (HATT) and the corresponding 2N-oxide were prepared. This study focuses on how the introduction of N-oxides in tetrazoles influences the thermal stability, energetic properties and sensitivities in this system. Therefore nitrogen-rich ionic derivatives (e.g. ammonium and hydroxylammonium) were synthesized and fully characterized using low temperature single crystal X ray diffraction. All compounds were investigated by NMR and vibrational (IR, Raman) spectroscopy, mass spectrometry, elemental analysis and DTA. The sensitivities toward impact, friction and electrical discharge were investigated using BAM standards and a small scale electrostatic discharge tester. The detonation parameters were calculated using the EXPLO5 V6.01 code. Heats of formation were computed by the atomization method based on CBS-4M electronic enthalpies. The N-oxides were compared to the corresponding compounds lacking the N-oxide moiety.

Investigations on the effect of 2N-oxides in aminohydroximoly-tetrazoles

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Keywords: tetrazole; N-oxide; crystal structure; nitrogen-rich.

Investigations on the density and performance increment of tetrazole-N-oxides exemplified by 5-aminohydroximoyl-tetrazoles are reported. For this purpose the new tetrazole derivative 5-aminohydroximoyl-2-hydroxytetrazole as well as 5-aminohydroximoyl-tetrazole were synthesized. In addition, their nitrogen-rich ionic derivatives (e.g. hydroxylammonium, ammonium, guanidinium) were synthesized and characterized using low temperature single crystal X-ray diffraction. All compounds were investigated by NMR and vibrational (IR, Raman) spectroscopy, mass spectrometry, elemental analysis and DTA. The sensitivities towards impact, friction and electrical discharge were investigated using BAM standards and a small scale electrostatic discharge tester. The detonation parameters were calculated using the EXPLO5 V6.01 code. Heats of formation were computed by the atomization method based on CBS-4M electronic enthalpies. The density, performance, thermal stability and sensitivity of the newly synthesized compounds were compared to each other to obtain a better understanding of the performance increment of the N-oxide group.

Quantification of thermal effect of a thermobaric detonation by infrared imaging technique

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Keywords: fire-ball; thermobaric explosive; thermography; infrared camera.

The aim of this work was to quantify the thermal effect of a thermobaric detonation by a thermography method in field tests, i.e. in static conditions. Thermobaric cast-cured PBX explosive test samples of two different masses were prepared. First, the following properties were determined for the examined explosive: density, detonation velocity and viscosity build-up in time. Experimental models were initiated by electro detonating cap and a plastic explosive booster. Detonation process and formation of the blast fireball were recorded by Phantom V9, TV high-speed camera, and by FLIR SC7200, infrared camera. Software "Altair" was used for data acquisition and analysis. Recordings of the IR scene of detonations were used to determine the temperature-time dependence at different distances from the detonation centre and the maximum developed temperatures. Also, the spatial distribution of the evolved heat in the blast fireball has been recorded. It was shown that it is possible to track and quantify the thermal effects by thermographic technique, but there is still much research to be done in this field.

Thermal decomposition of triazolo- and tetrazoloterazines

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Keywords: thermal decomposition; azoloterazines.

Thermal decomposition of 6-aminotrizolo[1,5-b]-1,2,4,5-tetrazine (ATrTz) and 6-amino-tetrazolo[1,5-b]-1,2,4,5-tetrazine (ATTz) in isothermal and non isothermal conditions has been studied. The decomposition of both substances follows a first-order reaction until high extent of decomposition. The kinetic data received is well described by straight lines in wide temperature intervals: k = $5.8*10^{10}$ exp(-17205/T), s-1(230-328 C) for ATrTz and k = $1.3*10^{25}$ exp(-29750/T), s-1(164-221 C) for ATTz. It was proposed a decomposition mechanism of these compounds.

Thermal decomposition of 5,5'-azotetrazole salts

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Keywords: salt of 5,5'-azotetrazole; thermal decomposition; decomposition; kinetic parameters.

Thermal decomposition of guanidinium, ammonium, melamine and sodium 5,5'-azotetrazole salts have been investigated. The kinetic parameters of the controlling chemical reaction have been estimated, and the detailed decomposition mechanism of 5,5'-azotetrazole salts has been proposed.

Acetone-water antisolvent crystallization of RDX and PETN in different crystallizers in the presence of stearic acid

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Keywords: RDX; PETN; spherical; crystal; sensitivity.

Crystallization of PETN and RDX from acetone solutions by addition of water as an antisolvent is favourite industrial process, used at many continuous or discontinuous production lines. Main advantage is high yield of a product, low price of an acetone and easy recovering of acetone. Disadvantage is poor quality of obtained crystals in some cases. This disadvantage should be suppressed by use of a suitable crystallizer and use of crystallization aids. It was found that use of a small addition (0.3-0.5%) of stearic acid causes formation of more spherical crystals with lower sensitivity of friction and impact. Crystallizers with baffles were preferred. Spherical high bulk density crystal material was tested for preparation of high solid filled plastic explosive and coated RDX as a composition A-5. Baffles were successfully tested in 2 m3 crystallizer and PETN or RDX-stearic acid explosives were inserted for advanced energetic material tests.

Applicability of model-free methods and thermal analysis data for studying decomposition kinetics of double base propellants

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Keywords: double base propellant; kinetics; model-free method; Ozawa method; Flynn-Wall method; nitroglycerine; nitrocellulose.

The non-isothermal differential scanning calorimetry (DSC) and thermogravimetry (TGA) data and iso-conversional model-free methods are often used to study kinetics of thermal decomposition of energetic materials. However, this approach is based on a number of requirements, which may limit its application. As the consequence of an uncritical use of thermal analysis data and model-free method in evaluation of kinetic parameters, the values of kinetic parameters reported in literature may differ considerable. In our previous studies on double base and single base propellants we have found that testing conditions (sample mass, heating rate, type of sample pan, etc.) significantly affect kinetic results. The effect was much more pronounced in the case of double base propellants, which also show existence of a discontinuity and slope change of the Ozawa plot. The results of this study show that for a correct kinetic analysis of thermal data for double base propellants one has to understand processes taking place in a complex decomposition mechanism and their effect on thermal analysis results, as well as to adjust experimental conditions so to satisfy necessary requirements for kinetic analysis as much as possible. For example, the sample self-heating effect may be eliminated using smaller sample masses (< 1 mg) and slower heating rates (< 3 oC min-1). The results show that for smaller sample masses and slower heating rates the activation energy calculated by Ozawa-Flynn-Wall method equals 173.8 kJ mol-1, while for faster heating rate it equals 151.6 kJ mol-1. It was shown by numerical simulation that such result is the consequence of both, complex decomposition mechanism and limitations of model-free kinetic methods.

A new method for the synthesis of triaminoguanidine salt of 3-nitro-1,2,4-triazol-5-one

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Keywords: triaminoguanidine salt of 3-nitro-1,2,4-triazol-5-one; nitrotriazolone; nitrotriazolone salts; NTO.

Many derivatives of 3-nitro-1,2,4-triazol-5-one (NTO) are described in last years, especially salts and complexes. Triaminoguanidine salt of 3-nitro-1,2,4-triazol-5-one (TAGNTO) is an important and prospective compound due to their high nitrogen content and reduced sensitivity for mechanical and shock initiation. We present the results of study on development of new method for synthesis of TAGNTO starting from NTO sodium salt and triaminoguanidine hydrochloride. Reactions were carried out in methanol in ambient and elevated temperatures. Solid products were collected by simple filtration, dried and weighed. The products were analyzed by using multinuclear NMR spectroscopy and DTA/TG techniques. Crystals shape were evaluated with images from optical microscope. It has been found that the optimal solvent for synthesis is methanol due to the solubility of by-product sodium chloride. TAGNTO forms stable hydrate which after dehydratation decomposes exothermically without melting at 201 °C.

Work ability of low-density emulsion based civil explosives

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Keywords: low-density explosives; work ability.

Requirements on properties of an explosive to be use in a blasting in special conditions like a blasting in nearness of a construction or buildings can be contradictory. Those explosives have to have enough amount of a released and transferred energy for rock breakage and on the other hand optimal part of shock energy for initial crushing. The low-density explosives are suitable for that kind of a blasting because of their properties. Mixtures based on an emulsion matrix with or without addition of a gas phase or expanded polystyrene had been tested. Work ability and performance of such explosive mixtures were measured by laboratory test methods.

Impact sensitivity test of liquid explosives

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Keywords: mechanical sensitivity; liquid explosives; initiation.

This paper presents the existing experimental and theoretical methods for mechanical sensitivity of liquid explosives. It is shown that the probability of explosion initiating by impact depends on the chemical nature of the substance and the various external characteristics. But the sensitivity of liquid explosive in the presence of gas bubbles increases many times as compared with the liquid without gas bubbles. Local hot spot in this case formed as a result of compression and heating of the gas inside the bubbles. If we consider that in the liquid as a result of convection, wave motion, shock, etc. gas bubbles are easily generated, the need to develop a method for determining sensitivity of liquid explosives to impact and a detailed study of the ignition explosives with bubbles is obvious. On a mathematical model of a single steam bubbles in the fluid theoretically considered the process of initiating explosive liquid systems to impact. For the experimental investigation, the well-known K-44 -II and the so-called appliance n^{o} 1were used. Instead of the metal cap in the standard method in this paper there was polyurethane foam cylindrical container with LHE, which is easily deforms by impact. A large number of tests with different liquid explosives were made. It was found that the test LHE to impact in appliance n^{o} 1 with polyurethane foam to a large extent reflect the real mechanical sensitivity due to the small loss of impact energy on the deformation of the metal cap, as well as the best differentiation LHE sensitivity due to the higher resolution method .

The use of thermite-incendiary compositions for burning of fairing of space launch vehicle

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Keywords: thermite-incendiary compositions.

The possibility of burning (as opposed to a mechanical destruction) of fairing of space launch vehicle (SLV) after having finished their mission directly at atmospheric part of the trajectory of their descent is considered. Different variants of thermite-incendiary compositions for their applying as part of the shell structure of fairing of SLV. Necessary amount of thermite-incendiary compositions have been evaluated, as well as losses of the payload mass. The effectiveness of the such a way to burn of fairing they fall on the Earth has been shown on the example of SLV "Soyuz-2.1 v".

Effect of an α-particle on various explosive materials

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Keywords: explosives; alpha particle; electrostatic interaction; DFT.

Effect of an α-particle on various explosive materials including TATB, FOX-7, TEX etc., is investigated using DFT approach at the level of B3LYP/6-31++G(d,p). For this purpose electrostatic model is adopted. Most of the explosive materials tested showed high distortion in the geometries in the presence of the alpha particle which should cause variation in performance. Although TATB deformed slightly without any bond cleavage, FOX-7 composite system attained a geometry in which the planes of nitro and amino groups are almost perpendicular to each other. Whereas TEX decomposed in the presence of α-particle. Some quantum chemical properties of these systems have been obtained and discussed.

The role of grain size and morphology on the sensitivity of e-HNIW

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Keywords: HNIW; impact sensitivity; friction sensitivity; decomposition; thermal stability.

In order to investigate the effects of grain size and morphology on the sensitivity of hexanitrohexaazaisowurtzitane (HNIW), HNIW samples with different grain sizes and morphology have been fabricated by recrystallization, respectively. The as-prepared HNIW was characterized by laser granularity measurement and scanning electron microscope (SEM). All samples were confirmed to be ε-form by X-ray diffraction (XRD) patterns and with high HPLC purities (>99%). The impact and friction sensitivity are tested, and the thermal stability of HNIW samples are also recorded by thermalgravity (TG) and differential scanning calorimetry (DSC). Results indicated that the impact sensitivity of HNIW decreased with the decrease of particle size and the friction sensitivity behaved on the contrary. Thermal stability of HNIW increased with grain size decreasing. Besides, HNIW with regular morphology had lower mechanical sensitivity and thermal stability than irregular crystals.

Comparison of the hot spots laser initiation effectiveness of the energetic materials by kilowatt and megawatt power pulses

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Keywords: laser initiation; hot spots; PETN.

Composite energetic materials explosion probability and induction period dependence on exposure was measured. Mixture of PETN with Al nanoparticles (ALEX, V-ALEX) and carbon black was used in experiments. Initiation of the explosion was carried out by using YAG: Nd laser LDPL10M (1064 nm, 532 nm, 10 ns, MW) and Yb fiber laser IRE-Polus YLR-150/1500-QCW-AC (1070 nm, 20ms, kW). Difference between the effectiveness of each additive for initiation by MW and kW sources of laser radiation was shown.

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