Abstracts of the 14th Seminar on

New Trends in Research of Energetic Materials

Pardubice, April 13–15, 2011

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

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Held at the University of Pardubice

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

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Preface

This is the fourteenth seminar *New Trends in Research of Energetic Materials (NTREM)* and the thirteenth in the series of seminars organised by the Institute of Energetic Materials (IEM) of the University of Pardubice. In the year that has passed from the thirteenth seminar, we lost some of the well-know personalities in the international community of people engaged in the field of energetic materials. The greatest loss for us is the demise of Professor Manfred Held in Feb. 8th, 2011; he was a very familiar person at international meetings and cooperation. Our whole community is now missing his unique contributions to Science of Detonics, and also his spontaneous help. Another loss, in particular for our Chinese colleagues from Chinese Academy of Engineering Physics (CAEP), is the death of Professor Haishan Dong in Feb. 3rd, 2011. Academician Dong became involved in chemistry of energetic materials and was one of the founders of Chinese Journal of Energetic Materials (HanNeng CaiLiao).

The previous Seminar was marked by the eruption of Island volcano Eyjafjallajökull; this eruption changed travelling and life plans of people all over the world and also prevented more than 70 our colleagues from participation in the 13th Seminar. The interest in this year's meeting in some ways compensates the last year's problem—the Organizational Committee of the 14th Seminar has received 111 full papers, which is a record in the whole history of our Seminars.

Realization of our Seminars would never be possible without the generous support from many institutions. The fourteenth NTREM seminar was financially supported by:

- U.S. Army Forward Element Command-Atlantic, Research Division, London, UK (conference grant)
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- STV Group, Rataje u Kroměříže, Czech Republic
- Faculty of Chemical Technology, Pardubice, Czech Republic
- OZM Reasearch, Hrochův Týnec, Czech Republic

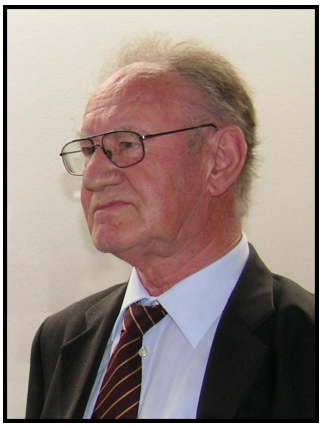
The efficient help in ensuring smooth and successful course of the meeting obtained from all these institutions is gratefully acknowledged. I greatly appreciate that, thanks to this support, all specifics of the previous Seminars can be maintained. It would be quite unfair not to mention personal effort of our foreign friends helping to find funding, publicize the Seminar abroad and personally participate in organizing activities during the event.

And traditionally, what should I add on the occasion of this 14th NTREM seminar? First of all, I would like to express the wish: May its proceedings be successful and may it bring inspiration and pieces of knowledge for use in further scientific research activities in the area of energetic materials, may it enable establishing new contacts and deepen the existing ones particularly between the young participants of this meeting. I wish for the participants to find a pleasant welcoming atmosphere throughout the seminar. Finally, I wish to thank the members of the Scientific Committee, the authors of all the submitted papers and, last but not least, you, the participants in this seminar, for its success and its influence on the continued success and growth of all future meetings at our University.

Pardubice, March 10, 2011

Svatopluk Zeman

Obituary



Prof. Dr. Manfred Held
★September 28, 1933, † February 8, 2011

He passed away by a sudden heart attack on February 8, 2011 at his 50th wedding day. Physicist of explosion who was an author of German version of the reactive armour (1967–1969) which was successfully used on Israeli tanks during the Arab-Israeli Conflict in 1982. Prof. Held performed all kind of investigations concerning shaped charge warhead systems and developed the "momentum method" for determining and characterizing blast effects. He was a respectable member of Scientific Committees of the International Seminars NTREM at the Faculty of Chemical Technology, University of Pardubice. Prof. Dr. Manfred Held was the first person in the International Balistics Society to be named a Ballistics Science Fellow.

The two-stage detonation propulsion model: exploring its intriguing trend-lines and equations

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Keywords: detonation; modeling.

This paper's goal is to reveal to students and young researchers issues that could be more thoroughly examined through new experimental work on and modeling of condensed explosive detonation.

The Two-Stage Detonation Propulsion Model was presented at the 9th NTREM as a means to identify, model, and explain effects occurring during the detonation of a condensed heterogeneous explosive that affect the explosive's measured and modeled performance. At the 10th and 11th NTREM, the model was used to reveal and describe issues well established by experiments described in scientific publications that could be explored differently using the model's methodology. Recently, other researchers have confirmed the importance of examining detonation-driven propulsion using a multi-stage model that might reveal the importance of processes occurring during the 1st stage.

The proposed paper uses information from the above-mentioned papers and additional scientific literature to offer students insight into research areas that now can be more thoroughly explored using modern experimental and computational capabilities: • Trend-lines describing the velocity of inert materials propelled during the 1st stage appear to also be capable of describing detonation wave propagation as well as how the inert material integrates the explosive's detonation-driven propulsion, • 1st propulsion stage effects may be principal factors affecting detonation propagation throughout an explosive charge, and • The equation describing motion during the 2nd propulsion stage can be integrated so as to conform to data taken during cylinder expansion tests as well as differentiated to explore effects remaining from 1st stage propulsion.

Recent efforts in tetrazine chemistry

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Keywords: high nitrogen; tetrazine.

The synthesis of high nitrogen energetic materials has been the focus of research at the Los Alamos National Laboratory for the past decade. Many of the molecules studied have been in the area of 1,2,4,5-tetrazine based heterocyclic materials. In this contribution, we will describe some recent efforts in our studies of tetrazine heterocycles. Several new materials have been prepared and the properties of these materials will be discussed.

Synthesis and reactivity of amino and nitrofuroxans

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Keywords: aminofuroxans; nirtofuroxans; synthesis; reactivity.

This communication covers the information about the most interest results of nitrogen-containing laboratory of ZIOC RAS in the field of the synthesis and reactivity of uncondensed amino- and nitrofuroxans.

Estimation of basic characteristics for some energetic polynitrogen compounds

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Keywords: polynitrogen compounds; oxidizer; enthalpy of formation; density.

Basing on earlier developed schemes for physical and chemical characteristics estimation, the enthalpies of formation, molecular crystals densities, detonation parameters, as well as sensitivity to different kinds of impact have been calculated. More than twenty compounds were investigated and some of them seem to be rather powerful. Among them there are about ten powerful explosives (e.g. dinitrodifuroxanyl, octanutrocubane, CL-20, azanitro-furazan, etc), low sensitive explosives (e.g. FOX-7, NTO, dinitropiperazine, diaminotrinitrobenzene, TATNB) and some hypothetic compounds (not synthesized yet) such as octaazacubane, octaazatetraen, tetranitrotetraazacubane etc. Energetic properties of the compounds were estimated for individual substances (acting as explosives or monopropellants), as well as for energetic compositions containing these compounds together with other ones, that are necessary for providing the requested parameters

Generic formulation of performance assessment quantities for stability, compatibility and ageing of energetic materials

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Keywords: performance quantities; generic assessment; stability; compatibility; ageing.

Most energetic materials decompose instrinsically under time-temperature loads. The decomposition can be enhanced by substances coming from the environment, for example as oxygen, water, acids, alkalines and substances containing transition elements. All energetic substances are characterized by an energy content, which is in total or partly released depending on the decomposition situation. For all energetic substances, neat or formulations, one can find limit values of residual energy content, which are necessary in order to fulfil the intended application of them. One generic aspect of defining assessment quantities relies therefore on the energy content. The absolute energy content or vice versa energy loss is however not general enough. The most general quantity in the discussed context is substance conversion. Very often the same substance conversion can be used for a lot of energetic materials designed for a defined application. For example, gun propellants should not surpass an energy loss defined conversion of 3 to 5 %. Otherwise the target picture is out of design. The basic definition of the three performance aspects stability, compatibility and ageing will be given on a conversion base for several measurement quantities often applied: energy loss, mass loss, gas generation. It is pointed out that the use of so-named intensive quantities like onset or peak maximum temperatures for assessing compatibility or ageing should be avoided when ever possible. They can be only a second choice compared to conversion related quantities. A further important aspect in comparing stability data is their transformation to other test conditions. This will be discussed and to follow the principle of Thermal Equivalent Load (TEL) is recommended.

Improved experimental procedure for the large scale gap-test

Chris Braithwaite, Jiri Pachman, Jiří Majzlík, David Williamson

SMF Group, Cavendish Laboratory, Cambridge University
University of Pardubice

Keywords: gap-test; experimental methods; Rowanex 3601.

A series of large scale gap-tests were conducted to calibrate the results for a ROWENEX 3601 donor charge to a stress scale. This was to resolve seeming discrepancies in previous experimental results. In this paper the authors suggest a number of pre-test investigations that allow for increased confidence in experimental results, and also some observations on the testing procedure itself.

Ageing behaviour of rocket propellant formulations with ADN as oxidizer

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Keywords: ADN based composite rocket propellants; ageing behaviour; DMA loss factor; molecular mobility regions in loss factor.

Characteristics and ageing of several ADN containing composite rocket propellant formulations were investigated. Binders have been GAP cured with BPS (bis-propargyl succinate) and Desmophene D2200 cured with Desmodur N3400. Comparisons are made with AP analogues, with formulations where HMX replaced Al, and with typical HTPB/Al/AP formulations. GAP-BPS/ADN/HMX and GAP-BPS/ADN/Al have low strength and low strain capability compared to HTPB/AP/Al-based propellants. Desmophene-bonded materials (ADN/Al, AP/Al, AP/HMX) have lower strain capabilities but higher strength values. The effectiveness of a bonding agent for ADN named HX-880 was studied, but a negligible effect on the mechanical properties was found and incompatibility with the ADN was observed. SEM analyses of the GAP-BPS/ADN formulations showed the presence of voids and a high porosity of the propellant formulations. With ageing the ADN formulations showed remarkable chemical decomposition (mass loss measurements evidenced an autocatalytic behaviour at above 60°C) and more severe or extended de-wetting between matrix and ADN prills. The glass transition temperatures determined by DMA for the GAP- and Desmophene-based formulations are about half as negative as the values of the AP/Al/HTPB-based propellants. The dynamic mechanical behaviour of the ADN formulations is different to the HTPB-based materials. Only one obvious peak in the loss factor curve was found instead of two. The filler (HMX or Al), oxidisers (AP or ADN) and curing agents (BPS or N3400) have influences on the glass transition temperature, peak broadness and apparent activation energy of the shift of peak temperature. The total peak of the GAP formulations is broader than the one of the Desmophene formulations. Lowering of Tg by the addition of AP was found. The fact that systematically the glass transition temperature is lower with AP compared to the ADN-based formulations can be explained with a stronger interaction between ADN and binder chains than between AP and binder chains.

Nitrocellulose's swelling process for liquid nitrate esters

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Keywords: nitrocellulose; kinetics of swelling; nitrate esters.

The interior ballistic performance of propellants can be significantly improved by the application of deterrents. The aim of this study is to examine influence of the deterrents on nitrocellulose. The kinetics of nitrocellulose spherical granule's swelling process was described. The swelling process was observed at different temperatures for three liquid nitrate esters: nitroglycerin, diethyleneglycol dinitrate and triethyleneglycol dinitrate. The relaxation time and diffusion coefficients were determined. The lowest value of diffusion coefficient was obtained for nitroglycerin, and the highest for diethyleneglycol dinitrate.

Derivatives of 3(5),4-dinitropyrazole as potential energetic plasticisers

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Keywords: synthesis; characterisation; energetic plasticiser; 3(5),4-dinitropyrazole.

The development of a pseudo-one pot synthesis of 3(5),4-dinitropyrazole enabled us to use it as a starting material for energetic plasticisers. Its acidic proton allowed simple derivatisation on one of the ring nitrogens. The thermal characteristics of two derivatives were evaluated. For instance, the N-allyl compound was a liquid with very low glass transition temperature, whereas the N-propargyl compound was a sticky solid at ambient temperature. The two compounds were both thermally stable according to STANAG 4582

Advanced plastic explosive based on bicyclo-HMX compared with Composition C4 and Semtex 10

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Keywords: plastic explosives; BCHMX; silicone; Composition C4; Semtex 10; sensitivity; detonation parameters.

BCHMX was studied as a plastic explosive bonded by Silicone matrix. For comparison the original plastic explosives, Composition C4 based on RDX as explosive filler and Semtex 10 based on PETN as explosive filler, were studied. Pure explosives used as active mate-rial in the plastic compositions were included as well. Sensitivity to impact and friction were measured. The thermal stability was studied using differential thermal analysis (DTA) and the outputs were evaluated by Kissinger method. The detonation velocity was measured experimentally and the detonation characteristics were calculated by means of CHEETAH code. On the basis of mutual comparison of all the obtained results, it was concluded that the new formulation has lower sensitivity to impact and friction than Com-position C4 and Semtex 10; also it has higher thermal stability. Detonation pressure and detonation energy of the new formulation were higher than the original plastic explosives used while its measured detonation velocity were at the same level of Composition C4.

The hydroxylammonium cation in tetrazole based energetic materials

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Ludwig-Maximilian University of Munich

Keywords: hydroxylamine; energetic materials; crystal structure; detonation parameters; sensitivity.

Due to its basicity, hydroxylamine was used to deprotonate several tetrazole derivatives bearing an acidic proton. Namely, the monodeprotonated 5-nitriminotetrazolate (1), dideprotonated 5-nitriminotetrazolate (2), 1-methyl-5-nitriminotetrazolate (3) and 2-methyl-5-nitraminotetrazolate salt (4) were synthesized. Further, the monodeprotonated (5) and dideprotonated bistetrazolylamine salt (6), a cocrystallization product of (5) with one equivalent of bistetrazolylamine (7) as well as the bis-deprotonated 5,5-bistetrazolate (8), the 5H-tetrazolate (9) and the tetrazole-5-carboxamide salt (10) were synthesized. All compounds except from 4 and 5 were fully characterized by single crystal X-ray diffraction. Additionally, 1 - 10 were characterized using vibrational spectroscopy (IR and Raman), multinuclear NMR spectroscopy, elemental analysis and DSC measurements. The heats of formation of 1 - 10 were calculated using the atomization method based on CBS-4M enthalpies. With these values and the experimental (X-ray) densities several detonation parameters such as the detonation pressure, velocity, energy and temperature were computed using the EXPLO5 code. In addition, the sensitivities towards impact, friction and electrical discharge were tested using the BAM drophammer, friction tester as well as a small scale electrical discharge device.

Excitation of PETN-charges with safe light-sensitive pyrotecnical compositions by incoherent light pulse sources

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Keywords: power-intensive compound; detonation; optical detonator; incoherent pulse light source.

An ongoing research programme at Russian Federal Nuclear Centre is devoted to numeri-cal and experimental studies of safe HE excitation by incoherent light pulses. The paper describes the main obtained results including experimental set-up, construction of high-voltage spark pulsed light sources, construction of optical detonators with a power-intensive compound, critical parameters of initiation energy and radiant power density. The experimental results obtained at initiating detonation in HE devices with compact in-coherent pulse light sources are presented. An application of this method for high-speed photorecording is discussed.

Definition of diversity for ignition of light-sensitive pyrotechnic composition pellets with roentgraph method

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Keywords: diversity; light-sensitive composition; pulsed x-ray method.

The paper outlines experimental set-up for studying diversity at the optical ignition of different devices containing a light-sensitive composition (ES-2). There are analyzed obtained radiographic results and discussed the possibility of using the composition in gasdynamic experiments needed in firing many shots to develop load design and diagnostics.

Energetic salts and chemistry of the nitrotetrazolate-2N-oxide anion

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Keywords: nitrotetrazolate-2N-oxide; HEDM.

The nitrotetrazolate-2N-oxide anion has been prepared by mild aqueous oxidation of easily prepared ammonium 5-nitrotetrazolate with commercially available oxone in high yields. The result of protonating 5-nitrotetrazolate-2N-oxide has been identified as a hydroxytetrazole, and the nitrogen-rich salts including ammonium, hydroxylammonium, guanidinium, aminoguanidinum, diaminoguanidinium, triaminoguanidinium, aminonitroguanidinium, diaminouronium, and aminotetrazolium have been prepared and characterized. Additionally, the products of alkylation have been studied. When compared to the nitrogen-rich salts of nitrotetrazolate, the nitrogen-rich salts of nitrotetrazolate-2N-oxide show superior energetic performance as calculated by the EXPLO5 computer code, using heats of formation calculated using the CBS-4M level of quantum mechanical theory. The impact, friction, and electrical spark sensitivities of the nitrogen-rich nitrotetrazolate-2N-oxides were measured and cover the whole range from sensitive to insensitive energetic materials.

Influence of structural and energetic factors on impact sensitivity of aromatic nitro compounds

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Keywords: aromatic nitro compounds; impact sensitivity; regression dependence.

There are two main approaches for the analysis of regularities of changing impact sensitivity for various explosives in dependence on some factors. The first one, phenomenological, is based on making physically substantiated reasonable models for the presentation of impact sensitivity dependences on the physicochemical properties of molecules determined using methods of quantum-chemical calculation. The second one, empirical, is based on making regression relations for the quite accurate description of impact sensitivity dependences on the composition and some structural characteristics of molecules. The combined method utilizing both of these approaches was used in this work when examining about 30 aromatic nitro compounds containing different substituting groups. Energetic characteristics of molecules, the main of which was the energy of nitro group dissociation, were determined in the realized calculations using the method of density functional theory (B3LYP/6-31+G(d)). Further the common regression dependence was built using the method of multiple regression analysis. Both the structural and energetic factors were used as independent variables in this analysis. The utilized combined approach reduced considerably the scatter of experimental data concerning the selected regression dependence, what allowed to estimate rather correctly the impact sensitivity of a great number of nitro compounds, for which there are no experimental data on impact sensitivity.

Energetic inks for screen printing

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Keywords: energetic inks; screen printing; shock tube detonators.

This research explores the use of printable energetic inks to fabricate shock tube ignitable detonator delaylines. The aim is to create an ink which is non-toxic, gasless, shock tube ignitable, and possesses a constant burn-rate which can be screen-printed. A screen print-able ink consists of a "pigment" (silicon and bismuth trioxide in this research), a resin (ni-trocellulose), a solvent and additives which prevent agglomeration, change its viscosity or quicken the drying process. The resin and the solvent form the ink-base to which other ink components can be added. In this research energetic powders are the main constituents, forming approximately 80 wt-% of the ink. Silicon is used as a fuel with bismuth trioxide as an oxidiser. PETN has been added to give further sensitivity to the compound. The current ink-base comprises a nitrocellulose-based resin and white spirit as a solvent. A Phantom Photo-Sonics camera has been used to record the combustion of the delayline. The meas-ured burn-rate for the above ink is 144 ± 3 ms/mm for a nominal ink thickness of 100 μm.

Computational study on all possible diamino-dinitropyrimidines and their mono and dioxide derivatives

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Keywords: diamino-dinitropyrimidines; explosives; detonation parameters; NICS.

Abstract: Diamino-dinitropyrimidines and their mono and dioxidized products have been subjected to theoretical analysis at the level of density functional theory with the application of B3LYP/6-31G(d,p) method of theory. In order judge the stabilities of the systems the electronic energies and the NICS data have been considered. 4,6diamine-2,5-dinitropyrimidine 11, 2,6-diamino-4,5-dinitropyrimidine-1-oxide 8a and 2,4-diamino-5,6-dinitropyrimidine-1,3-dioxide 8c are calculated to be the most stable structures among pyrimidines, mono and dioxide derivatives, respectively. As these compounds are potential high energy density materials, their detonation parameters have also been reported herein, together with bond dissociation energies regarding to homolytic bond dissociation of the C-NO2 bond. The reported data suggest that these compounds (8-11b) are all possible potential candidates for insensitive but effective explosive materials.

Continuous aerobic degradation of dinitrotoluenes in packed bed reactors

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Keywords: packed bed reactors; immobilized mixed culture; dinitrotoluenes; degradation rate and efficiency.

Continuous 2,4-dinitrotoluene and 2,6-dinitrotoluene degradation by a mixed microbial culture immobilized on three different packing materials was stud-ied. The packing materials applied were: expanded slate, perlite, polyurethane foam (PUF). Experiments were carried out in three packed bed reactors with a concurrent water-air flow under conditions of oxygen in excess. The loading rate was varied by changing the inlet 2,4-DNT or 2,6-DNT concentrations. The most efficient 2,4-DNT biodegradation as a single substrate was achieved with the PUF packing. While treating a mixture of DNTs, the removal effi-ciency of 2,4-DNT was strongly suppressed whereas that of 2,6-DNT in-creased.

Multi-person assessment of RDX crystal morphology using the RS-RDX round robin method

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Keywords: RDX; crystal morphology; microscopy; shock sensitivity.

The crystal morphology of RDX has been linked to the shock sensitivity of polymer bonded explosives. During the reduced sensitivity RDX Round Robin (R4) study, crystal morphology was assessed using contrasting fluid optical microscopy and a scoring system. This method was able to show a difference between different crystal lots. However the method was very subjective and large variations between assessments were seen. The procedure was repeated by the author, a larger number of crystals from each batch were examined. Similar results were obtained. To gain a better understanding of how subjective/variable the method is, the micrographs obtained were then assessed by a larger number of (unskilled) analysts and the results compared. The results showed reasonable agreement between assessors. Unprocessed type II RDX lots were on average assessed to be more angular, but also had the most variation between assessors. There was closer agreement between type I/RS-RDX lots which were assessed to be smoother. The method was found to be time consuming by many of the assessors.

First-principles hydrostatic compression study of phase I of AP and alpha-, epsilon- and gamma- polymorphs of RDX

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Keywords: ammonium perchlorate; RDX; DFT-D; hydrostatic compression.

We have performed density functional theory (DFT) calculations to study the hydrostatic compression of phase I of ammonium perchlorate (AP) and the alpha-, gamma-, and epsilon- polymorphs of cyclotrimethylenetrinitramine (RDX). A comparison of the performance of different DFT dispersion- correction schemes in calculating crystal geometries and vibrational frequencies at high pressure has been performed for AP. Using 'on-the-fly' (OTF) pseudopotentials, the experimental compression behaviour of phase I AP has been reproduced for all DFT dispersion correction schemes studied. DFT-D calculations on the alpha-form of RDX reproduced the lattice energy in exceptional agreement with experiment, thus the lattice energy of the metastable beta-form was confidently predicted. The calculated lattice parameters and unit cell volumes for alpha-, gamma-, and epsilon-RDX polymorphs were in excellent agreement with experiment both at ambient and at elevated hydrostatic pressures. Comprehensive vibrational mode calculations (including symmetry) as a function of pressure have been performed with the frequency of all predicted internal modes, again in good agreement to experiment.

Replacing the equations of Fano and Fisher for cased charge blast equivalence

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Keywords: munition; blast; cased; fragmentation; impulse; Gurney.

The initial velocity of casing fragments from bombs, shells etc. was first calculated by R.W. Gurney in 1943. This derivation was based on a reasonable simplification of the casing and gas dynamics. Subsequently, Gurney's wartime co-worker, U. Fano, issued a further report on the blast equivalence of cased explosive charges, i.e. the blast impulse they deliver as a fraction of the impulse from the same charge uncased. Fano claimed to have calculated the proportion of kinetic energy remaining with the explosive gases following energy partition with the casing. This presentation will show that Fano's equation for cased charge blast equivalence is inconsistent with Gurney's reasonable physical model, as is a further equation by Fisher. The presenter will draw attention to an equation recently published, which gives similar predictions to that of Fisher, while being consistent with Gurney's original derivation. Also, based on CONWEP data, the presenter has established for the first time that the use of such equations for cased charge blast equivalence is valid. Furthermore, by combining Gurney's kinetic energy equation with G.I. Taylor's equation for case fracture strain, a casing-gas energy balance at fracture can be obtained. A comparison with historic AWE cased charge blast impulse data shows reasonable agreement, but further experimental data are required.

Some physico-chemical properties of products of chemical transformation of 2,4,6-trinitrotoluene

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Keywords: trinitrotoluene; chemical transformation; quantum chemical calculations; spectral characteristics.

Technology of the process of transformation of trinitrotoluene (TNT) into products of civil needs is discussed. Substitution of nitro-groups by OH-groups with further nitrozation leads to formation of a dinitrozo-substituted methylfloroglucine which pocessess good dying properties. The tautomeric transformations, spectroscopic characteristics and features of structure are discussed with the help of spectroscopy, X-ray analysis on single crystals and quantum-chemical calculations.

Physicochemical properties of condensed systems based on 5,6-(3',4'-furasano)-1,2,3,4-tetrasine-1,3-dioxide

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Keywords: 5,6-(3',4'-furasano)-1,2,3,4-tetrasine-1,3-dioxide.

5,6-(3',4'-furasano)-1,2,3,4-tetrasine-1,3-dioxide (C2N6O3, FTDO) is a promising energetic material. It has a formation enthalpy of 1000 cal/g and therefore is unstable and very sensitive. To lower the sensitivity FTDO is crystallized together with linear nitramine 2,4-dinitro-2,4-diazapentane (S3H8N4O4, DNP) in different ratios. Combustion of these mixtures is unstable at high pressures. The threshold of stable combustion is dependent on the ways by which they are prepared. Thus, the study of physicochemical properties of condensed systems is needed to understand the cause of instability and try to overcome it. In this study the following methods have been applied: IR-spectroscopy, UV-Vis-spectroscopy, X-ray diffraction, computed X-ray microscopy and tomography, optical microscopy. Diffraction and tomography allowed an examination of internal structure of condensed systems without destroying them. Using these methods the crystallites sizes, pores sizes and integral porosity were defined as well as dependence of these characteristics on preparation conditions. UV-Vis-spectroscopy for this particular system allows determining FTDO/DNP ratio with 1% accuracy using only 1 mg samples. This study showed that components (FTDO and DNP) are not evenly distributed in the crystallized mixture. Thus, the complex of available methods allows us to fully characterize samples of condensed systems before combustion experiments. In future this may help to understand how physicochemical properties of condensed systems influence the combustion of condensed systems.

Ignition of light-sensitive compositions with explosive thermochemical sources

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Keywords: light-sensitive pyrotechnic composition; ignition; explosive thermochemical source.

The paper presents experimental set-up and results on ignition of light-sensitive pyrotechnic compositions on the base of perchlorate cuprum and perchlorate hydrargyrum (II) by radiation of explosive thermochemical sources containing HE and dispersed aluminum powder. The peculiarities of such ignition is analyzed.

Blasting fumes in underground workings

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Keywords: blasting fumes; gases; carbon monoxide; carbon dioxide; nitrogen monoxide; nitrogen dioxide.

It is in the nature of explosives to form large quantities of gas during detonation. This gas mixture, the so called “blasting fumes”, are mainly made up of reaction products of the used explosive and, as described in this contribution, follow some common principles. Modern commercial explosives are mixtures of compounds containing four basic elements: carbon, nitrogen, hydrogen and oxygen. According to the theoretical detonation reaction of an explosive, only non-toxic gaseous products should be formed during the complete decomposition, namely CO2, H2O and N2. In reality, however, besides the non-toxic gases, also large amounts of fume components of varying toxicity are formed. These products of incomplete composition are mainly carbon monoxide (CO), nitrogen monoxide (NO), nitrogen dioxide (NO2) and ammonia (NH3). In addition, also volatile organic compounds and non-detonated portions of the explosive can be found in the fumes. These blasting fumes which are formed in every blast can, depending on the operation site, have rather disturbing influence on the workings around the blast. While fumes from a surface mine blast have minor relevance on the work, in underground mining the existence of blasting fumes causes a great problem. On one hand, blasting fumes have an annoying and irritating smell while on the other hand, the toxicity of some fume components, especially CO and NOx, can pose a considerable health threat on the underground work force. This contribution is focusing on one of the research fields of the Chair of Mining Engineering, discussing problems with blasting fumes in underground workings. Several research reports from our institute as well as articles from institutions around the world are summarized and compared with practical tests from blasting chambers and production blasts. The research works show that the formation of blasting fumes is mainly influenced by the mechanic and chemical conditions during detonation of the explosive. Further, after detonation reaction processes of remaining explosive and formed fumes with the environment play a major role in the formation of blasting fumes.

Co-crystallisation of energetic materials: a step towards tailored munitions?

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Keywords: co-crystallisation; HMX; CL-20.

Co-crystals, which have been defined as "multi-component molecular crystals" [1], have been used extensively in attempts to improve upon the performance of pharmaceutical compounds [2]. It has become clear that a wide range of pharmaceutical co-crystals can be rationally designed using crystal engineering, affording new intellectual property and enhanced properties, such as dissolution rate and relative stability [3]. Furthermore, co-crystallisation experiments are of academic importance as they provide an insight into the competitive intermolecular interactions that occur during crystallisation. It is our aim to extend these studies to co-crystallisation of energetic materials, firstly with a range of readily available organic molecules before devising a strategy to tailor these systems to improve operational performance. Our current studies are focussed on co-crystallisation of HMX and CL-20 with a range of organic molecules. By using a combination of single crystal and powder X-ray diffraction and variable temperature Raman spectroscopy we have been able to elucidate not only the structures of these novel materials but also their stabilities with respect to temperature and pressure. Furthermore, preliminary tests suggest that co-crystallisation can have a dramatic effect on sensitivity, thereby allowing the modification of existing energetic materials to produce enhanced munitions. We present a summary of this work and outline our current strategies for extending these techniques to other energetic materials. [1] A.D. Bond, CrystEngComm, 2007, 9, 833. [2] N. Schultheiss and A. Newman, Cryst. Growth Des., 2009, 9, 2950. [3] Ö. Almarsson and M.J. Zaworotko, Chem. Commun., 2004, 17, 1889.

Prediction of impact sensitivity of nitro energetic compounds using QSPR approachs

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Keywords: impact sensitivity; QSPR; nitro energetic compounds; DFT.

The new European regulation of chemicals REACH aiming to reinforce the control of risks from chemicals in Europe entered into force in 2007. It may require the reassessment of hazardous properties for up to 140000 substances until 2018. However, the complete experimental characterization of (eco)toxicological and physico-chemical properties is time-consuming, costly and sometimes simply not feasible at the R&D stage. Therefore, the development of validated alternative methods for assessing hazardous properties of chemicals is promoted in REACH.

The present work focuses on the development and validation of Quantitative Structure-Property Relationships (QSPR) models to predict the impact sensitivity of potentially explosive molecules (nitroaromatics, nitroaliphatics and nitramines,. . .).

To set up appropriate relationships between different molecular descriptors of these compounds and their impact sensitivity, an original approach associating the QSPR method to quantum chemical calculations was developed. More than 300 molecular descriptors (constitutional, topological, geometrical, quantum chemical) were calculated using CodessaPro software from calculated molecular structures, optimized with the Density Functional Theory (DFT) in Gaussian03 package. Theses descriptors were integrated into statistical multilinear regressions to link them quantitatively to experimental data obtained on the impact sensitivity property. In order to validate models according to the OECD principles for the use of QSPRs in a regulatory context, models were developed on a training dataset and their predictivity was verified on a validation dataset. Once validated, models are expected to be integrated into a global tool to estimate explosibility hazards of substances (for classification purposes) and the need for further experimental testing.

Estimation of the Lee-Tarver reactive flow model parameters for an ammonium nitrate based emulsion explosive

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Keywords: genetic algorithm; emulsion explosive; Lee-Tarver reactive flow model.

The use of explosive generated SW for powder processing is receiving a renewed attention as an alternative route capable to overcome the traditional problems of the classical techniques for the processing of nanocrystalline, super-hard, high-Tc superconducting, metastable highly-alloyed or amorphous powdered materials. For this kind of situation computer simulations are of an inestimable importance since they allow a significant reduction of the experimental tests needed to be performed in order to achieve the optimal configuration parameters. However, while for the great majority of the materials and of the military explosives the value of the input parameters of the material models and of the equation of sate [EoS] is known, for powdered materials and for non-ideal (industrial) explosives, like the ones normally used in the compaction processes, those parameters are often not known. In this work, a real coded genetic algorithm methodology that has been developed for the estimation of the parameters of the reaction rate equation of the Lee-Tarver reactive flow model is described in detail. This methodology allows, in a single optimization procedure, using only one experimental result and without the need of any starting solution, to seek for the fifteen parameters of the reaction rate equation that fit the numerical to the experimental results. Mass averaging and the Plate-Gap Model have been used for the determination of the shock data used in the unreacted explosive JWL EoS assessment and the thermochemical code THOR retrieved the data used in the detonation products JWL EoS assessment. The developed methodology was applied for the estimation of the referred parameters for an ammonium nitrate based emulsion explosive using PMMA embedded manganin gauge pressure-time data. The obtained parameters allow a reasonable good de-scription of the experimental data and show some peculiarities arising from the intrinsic nature of this kind of composite explosive.

Decomposition and combustion of 4,4'-bis[4-aminofurazanyl-3-azoxy]-3,3'-azofurazan and its macrocyclic analog

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Keywords: azofurazan; azoxyfurazan; macrocyclic azoxyfurazan; decomposition; combustion; mechanism.

Energetic azofurazan and azoxyfurazan compounds are very important class of furazan-based energetic materials, which have received much attention due to their favorable properties such as high energy density, low sensitivity, good heat stability, and high percentage of nitrogen content. The goal of the present work was comparative study of representatives of polyazo and azoxyfurazans: 4,4'-bis[4-aminofurazan-3-yl-azoxy]-3,3'-azofurazan (DAAAzF) and its macrocyclic analog tetra(diazenoxide furazan) (TOATF). Thermal decomposition of these explosives, DAAAzF and TOATF, has been investigated under isothermal and non isothermal conditions using the thin-walled glass manometer of the compensation type and DSC, correspondingly. Both polyfurazans are thermally stable compounds. The comparison of the DAAAzF and TOATF decomposition rate constants obtained under isothermal conditions in liquid state shows that thermal stability of macrocyclic polyfyrazan significantly exceeds not only stability of linear analog, but also stability of RDX and HMX. It is interesting to note that activation energy of TOATF decomposition (50 kcal/mole) is close to the strength of the weakest bond in macrocycle, whereas activation energy of DAAAzF decomposition (31 kcal/mole) is characteristic for concert mechanism of azoxygroup removal. Burn rate characteristics of DAAAzF and TOATF in the form of samples pressed into acrylic tubes of 4 mm diameter or in the form of pellets 1h2h10 mm have been investigated in the pressure interval of 0.05-15 MPa. Burning rates of both DAAAzF and TOATF are faster as compared with HMX, and burning rate of TOATF exceeds burning rate of CL-20. The temperature distribution in the combustion waves of DAAAzF and TOATF has been measured with help of thin thermocouples. The thermocouple measurements showed that leading reaction on combustion of DAAAzF and TOATF is located the condensed phase and their burning rates are defined by kinetics of decomposition at the surface temperature. Kinetics of DAAAzF and TOATF decomposition at 500-700 S calculated by using a condensed-phase combustion model are in a good agreement with kinetics data obtained in melt or solution at 235-270 S.

Thermal initiation of consolidated reactive nanocomposite powders

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Keywords: thermite; ignition.

Interest in improved and multifunctional energetic components has led to development of new reactive materials. These materials are tailored to provide the energetic performance as well as a secondary function. In reactive structures, the material provides a highly exothermic reaction as well as functioning as a structural component. In this study reactive nanocomposite powders prepared by arrested reactive milling are consolidated into cylindrical pellets of diameter 0.635 cm by uniaxial die compaction to up to 99% of their theoretical maximum density. Pellets made of different thermite compositions including Al-MoO3 Al-Fe2O3, and Al-Bi2O3 are placed in an enclosed chamber and ignited by a CO2 laser. The ignition delay and combustion pressures are measured. Ignition delays are measured as a function of laser power and material composition. In addition, the effect of pellet density on the ignition delay is identified for the same material and a fixed laser power. A heat transfer model describing laser heating of a cylindrical pellet is implemented into a numerical code. The exothermic chemical reaction leading to ignition is represented by a zero-order Arrhenius reaction term with the activation energy identified from earlier experiments with non-consolidated nanocomposite thermite powders. The calculations are in good agreement with the measurements suggesting that the proposed ignition model describes adequately the thermal initiation of the consolidated reactive samples.

Effects of additives on the crystal morphology of TATB

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Keywords: TATB; recrystallization; additives; crystal morphology; hydrogen bond; Π-stacking interaction.

The morphology controlling of TATB (1,3,5-triamino-2,4,6-trinitrobenzene) can help to control preferred orientation and anisotropic expansion of TATB based PBXs, as well as to improve crystal quality, desensitizing efficiency, packing density, and even explosive energy. This paper investigates the effects of additives on the crystal morphology of TATB. It is shown that the additives that can form hydrogen bonds with TATB molecules lead to near-spherical crystals, while additives with big conjugated π-bonds lead to platy crystals. This can attribute to the different interaction between the solvents and different face of TATB crystals. The solvents with hydrogen bond acceptor and donor are easy to attach to the 100 and 010 face, and will restrict the crystal growth of these faces. Subsequently, they will be more morphology important and have stronger diffraction peak in the XRD pattern. By π-staking interaction, the additives containing aromatic π-bonds can restrict the crystal growth of 001 face, and make it the most morphological important crystal face, only whose diffraction peak can be observed in the XRD patterns. The results of this investigation will provide some guide for the crystal morphology controlling of TATB.

Assessment of factors effecting stabiliser extraction from nitrocellulose based propellants

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Keywords: stabilizer extraction; nitrocellulose; 2-NDPA; UV-VIS absorption; AOP-48.

Ensuring propellants in service are safe for use, is critically important. The principal method for determining the remaining service life involves the assessment of stabiliser concentration. This paper uses high performance liquid chromatography and UV-visible spectrometry to review and assesses the effectiveness of the stabiliser extraction method detailed in AOP 48. Investigating how a number of factors; solvent type, temperature, rate of shaking or stirring effect the stabiliser extraction rate, in order to better understand the kinetics of the process.

The use of accelerating rate calorimetry to understand the ageing behaviour of complex hybrid propellants

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Keywords: acelerating rate calorimetry; propellants.

Propellant compositions with high energy characteristics are required to meet the demanding performance requirements of many current and proposed future weapons systems. This can be achieved through formulations which incorporate mixtures of nitrate esters, ammonium perchlorate, polymeric binder, aluminium and nitramine high explosive materials. In the past, it has been found that some propellants of this type have had a tendency to exhibit rapid transition to explosive behaviour during ageing tests at elevated temperatures as opposed a more controlled thermal runaway process observed in simple nitrate ester propellants. This paper describes the use of Accelerating Rate Calorimetry (ARC) and chemical analysis to understand the ageing phenomena of such propellants, particularly with regards to their thermal behaviour.

Synthesis, characterization and properties of 5-nitraminotetrazole high nitrogen salts

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Keywords: 5-nitraminotetrazole salts; structural characterization; thermal analysis; sensitivity.

Three high-nitrogen energetic 5-nitroamino-tetrazole salts, (NH2NH2)+(NATZ)-Œ0.5H2O, (CHZ)+(NATZ)- and (en)+(NATZ)-, were synthesized. The nitrogen-rich salts were characterized by elemental analysis and infrared spectra techniques. In addition, the single crystal of (CHZ)+(NATZ)- was cultured and were determined by X-ray single crystal diffraction analysis. The crystal of (CHZ)+(NATZ)- belonged to the monoclinic system, space group Pn, with cell parameters: a=0.37389(1) nm, b=1.2396(5) nm, c=0.8699(4) nm, β=92.212(7)o, V=0.4029(3) nm3, Z=2, ρcacl=1.815 g/cm3, R1=0.0287, wR2(all data)=0.0564. The thermal stabilities of 5-nitroaminotetrazole salts were investigated using differential scanning calorimetry (DSC) and thermo-gravimentry - differential thermo-gravimetry (TG-DTG) techniques. At a heating rate of 10K/min, the thermal decomposition process of (NH2NH2)+(NATZ)-Œ0.5H2O consists of one endothermic peak without residues, while the others consist of one endothermic peak and one exothermic peak . The sensitivities properties showed that the impact sensitivity and friction sensitivity were higher, while the flame sensitivity was lower. So they can be used as promising energetic materials in ammunition and civil applications.

Influence of pad or air gap between the high explosive and flyer

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Keywords: detonation; plate push; pad; air gap.

Numerical simulations of plate push by JOB-9003 were carried with two dimensional lagragian codes. A thin pad or air gap was set between the high explosive and flyer. Different influence on the flyer motion induced by the pad or air gap is discussed in one dimensional detonation and two dimensional sliding detonation separately. One dimensional detonation plate push results show that the kinetic energy of the flyer with pad is higher than that of flyer with air gap at the early stage, but it turns to be lower in the following process. The reason is that pad between the HE and the flyer improves the ingoing pressure from the HE detonation in the flyer, and the flyer with pad moves faster after the HE detonated. But the reflected rarefaction wave into the HE product in the case of pad between the flyer and the HE is also stronger than that of air gap, so the HE product pressure in the pad case is lower than that in air gap case. Then that could explain the trend of kinetic energy in one dimension. Two dimensional results don't show the same trend in the flyers' kinetic energy as that in one dimension. The flyer with pad moves faster than that with air gap all the time since the pad between the flyer and HE enhance the ingoing pressure in the flyer and the rarefaction wave draw less effect to the product in the moving direction of the flyer because the detonation wave is almost perpendicular to the flyer in two dimensional sliding detonation. This conclusion could be the interest of detonation system designers.

Interfacial interaction between double (010) faces of β-HMX

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Keywords: interfacial interaction; explosive crystal; compression; stretching; shear; twist.

The interfacial interaction between double (010) faces of β-HMX was computationally discussed for the first time to simulate an explosive crystal against external mechanical stimuli probably causing some interfacial movements including compression, stretching rupture, shear slide, and twist. The results show that: (1) in the equilibrium structure of the HMX crystal, the distance between two neighboring layers close to the crystal surface is longer than that in the crystal bulk, showing the looser molecules on or near the surface; (2) a point of inflection of the distance between the centroids of the two blocks (d) composing the (010) interface appears at d=3.3 Å, where there are the biggest surface areas of the interfacial HMX molecules and three extremums of van der Waals, valence and electrostatic interaction energy (ΔE), respectively. And it also leads to non-monotonous changes of ΔE-d correlation of valence interaction during both shear sliding and twisting; (3) the highest sliding and twisting barriers along the (010) face in case of no crystal crack, can make each interfacial HMX molecule share averagely the increased energy 48 and 140 kJ/mol, respectively. From a comparison of these increased energy with the apparent activation energy of thermal decomposition of HMX crystal, 140 kJ/mol, we deduce that the shear sliding along (010) face without crystal rupture is probably allowable, but the twisting is forbidden; and (4) the change of total interaction energy during sliding and twisting is dominated by that of van der Waals interaction energy.

Numerical simulation of STEVEN impact test

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Keywords: Steven test; detonation; Lee-Tarver reactive flow model.

Detonation sensitivity is important index for measuring initial capability high explosive, Steven test is one of the basic tests about gauging and has greatly increased the fundamental knowledge of practical predictions of impact safety hazards. The ignition and growth (I&G) reactive flow model is a constitutive kinetics model that has been used to simulation for Steven test. In this paper, we describe a modified form of Lee-Tarver reactive flow model , Lagrange model and elastoplasticity hydrodynamics model. It is better suited for test data.

Nitration of aromatic compounds with using solid catalysts: $H_3PO_4/MoO_3/SiO_2$ and $H_3PO_4/WO_3/SiO_2$

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Keywords: nitration; aromatic nitro compounds; solid acid.

Aromatic nitro compounds are widely used in the chemical industry as intermediates in synthesis of drugs, chemical fertilizers, plastics, dyestuffs. Furthermore, they are used as explosives or substrates in explosives manufacture. Nitro compounds are additives in propellants, gunpowder and explosive mining materials. Such compounds are nitro derivatives of toluene, xylene, chlorobenzene, naphthalene, phenol and anthracene. Aromatic nitro compounds are obtained in nitration process with using a nitrating mixture that commonly is a mixture of HNO3/H2SO4. However, there is a need to remove H2SO4 from chemical process because of ecological reasons. Moreover, very often there is a need to obtain nitro compounds with high purity, which is very difficult during nitration with using HNO3/H2SO4. In connection with that it is important to find other effective catalysts that enable nitration in mild conditions. Our work is focussed on the catalysts in the form of metal oxides (Mo, W) deposited on silica gel and modified by H3PO4, that are very effective in aromatic nitration. The catalysts enable nitration in mild conditions with lower amounts of HNO3. They have also ability to introduce two nitro groups in one stage. Products of nitration are not contaminated by H2SO4. Furthermore, described catalysts are effective in nitration in flow process without using extra solvent.

Absorption spectra of PETN and efficiency of laser initiation

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Keywords: PETN; spectra; absorption; laser; initiation.

A comparative study of the efficiency of the laser initiation of PETN by the first and second harmonics (1060 and 530 nm) of a neodymium-doped phosphate glass laser was performed. A significant difference in the efficiency of PETN initiation by the different harmonics was revealed: as the initial temperature of the sample increased from 373 to 450 K, the threshold initiation fluency decreased from 3.0 to 0.5 J/cm^2; at the same time, the second harmonic failed to initiate PETN even at a fluency of 10 J/cm^2. The absorption spectrum of PETN was found to have a weak absorption band with a maximum at λm = 1020 nm. It was assumed that the high efficiency of initiation by the first harmonic is associated with light absorption (photoinitiation) by this band.

New NMR data of molecular dynamic of nitroguanidine

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Keywords: NMR spectroscopy; nitrimines; nitroguanidine.

The 1H NMR spectra of nitroguanidine has been investigated in solution in the temperature range of -44 to +48C. The degenerate rearrangement of nitroguanidine has been discovered first time.

Some properties of 1-(2,4,6-trinitrophenyl)-1,2-dinitroguanidine

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Keywords: high explosives; nitrimines; nitroguanidine; nitrocompounds.

Sensitivity of 1-(2,4,6-trinitrophenyl)-1,2-dinitroguanidine to thermal and mechanical initiation is investigated. This compound is a powerful high explosive but it has the high level of impact sensitivity (more than PETN) and the comparatively low temperature of flash.

Synthesis and some chemical properties of amidrazone of dinitroacetic acid

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Keywords: amidrazone of dinitroacetic acid; 1,1-diamino-2,2-dinitroethylene; FOX-7.

1,1-diamino-2,2-dinitroethylene can easy be converted to 1-amino-1-hydrazino-2,2-dinitroethylene (amidrazone of dinitroacetic acide) by the action of hydrazine in water solutions. Reactivity of amidrazone moiety of 1-amino-1-hydrazino-2,2-dinitroethylene is discussed. 1-amino-1-hydrazino-2,2-dinitroethylene may be used as precursor for some heterocyclic systems including dinitromethylene moiety.

Synthesis of mono-dinitromethyl-1,3,5-triazine salts

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Keywords: mono-dinitromethyl-1,3,5-triazine salts; denitration of mono-trinitromethyl-1,3,5-triazines.

Synthesis of mono-dinitromethyl-1,3,5-triazine salts containing amino-, alkoxy- and aryloxy functionality was reported. Method is based on denitration of mono-trinitromethyl-1,3,5-triazines. Formation of by-products in this method is discussed.

New energetic nitrogen rich polymers

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Keywords: energetic polymer; nitrogen rich polymer; vinyl group; tetrazoles; triazoles.

New energetic nitrogen rich polymers, based on vinyl groups, were synthesized using common procedures. The point of interest was the introduction of tetrazole containing moieties. The polymers were characterized by multinuclear magnetic resonace study (1H, 13C), vibrational spectroscopy (IR) and elemental analysis. The energetic properties of the polymers were investigated using differential scanning calorimetry and bomb calorimetric measurements along with calculations using the EXPLO5 software.

Investigation on PPX polymers models and their adsorption to gas molecules

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Keywords: poly-para-xylylene; Grand Canonical Monte Carlo; adsorption; gas molecular.

The status of gas molecules in PPX polymers (poly (p - xylylene), parylene) is important in coating areas of the forces electron plate, such as structural establishment, gas site and energy transfer. In this paper, molecular mechanics (MM) and NVT+NPT-annealing simulations had been applied to build the PPX polymers models including PPX N, PPX C and PPX D. The quantity and site of gas molecules in PPX polymers were calculated using Grand Canonical Monte Carlo (GCMC) with COMPASS force filed over a range of temperatures (150 – 450 K). The corresponding energy was investigated using adsorption energy formula. The average adsorption numbers and energy were found.

EXPLONIX - new portable detection device

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Keywords: portable detection device; explosive detection; explosive traces.

The EXPLONIX system is new technolology for detection and analysis of explosive traces.It is capable to detect a wide range of explosive materials, including non-volatile substances like HMX. Explosive detection is based on chemiluminescence principle which allows reliable results and fast responce. Instrument is equiped by three devices suitable for sampling from various surfaces. Direct vapor mode sampling is wide used one-second method for sampling volatile substances like TNT or tagants. InfraRed continous vapour mode sampling device ekes direct vapor mode sampling method. It is build-in system for non-contact sampling using thermal energy for desorbing non-volatile samples from surface or from special sampling strips. The last included sampling method uses special needle for collecting samples from rugged relief. This needle is inserted directly into instrument where sample is desorbed.

Detonation parameters calculations of different high explosives using computer program XW

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Keywords: detonation; numerical modelling; detonation parameters; high explosives.

The computer program XW is developed based on thermochemical numerical model of detonation. The XW is developed in graphical user interface using the Delphy® 6.0 application, and can be successfully used on modern personal computers with WindowsXP® OS. The numerical model of detonation uses BKW equation of state with different sets of parameters. The detonation products are calculated using the free-energy minimization criterion. The XW calculation results of detonation parameters for different high explosives are compared with experimental data and calculation results using other numerical models. The analyzed XW calculation results of detonation parameters have good correlation with experimental data.

Experimentally determined detonation velocities of new secondary explosives

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Keywords: booster charge; detonation parameters; detonation velocity; fiber optic technique; secondary explosives.

The detonation velocities of several compounds with possible application as new secondary explosives were experimentally determined in an OZM laboratory detonation chamber (model KV-250) using the fiber optic technique. The investigated explosives are 1-amino-3-nitroguanidine (1), diaminouronium nitrate (2), dihydroxylammonium 5,5-bistetrazolate (3), hydroxylammonium 5-nitriminotetrazolate (4), oxalylhydrazide nitrate (5) and 1,3,5-triaminoguanidinium 1-methyl-5-nitriminotetrazolate (6). The compounds were synthesized on a 20 g scale, loaded into a PE tube and initiated with an electrically ignited detonator containing PETN and RDX. If necessary, PETN was used as a booster charge. The measured detonation velocity was recorded using the OZM detonating velocity measuring system EXPLOMET-FO-2000 and compared to the values that were calculated using the EXPLO5 code and the loading density of the respective compound.

Regulation of PETN sensibility by Al nanoparticle additives during laser initiation

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Keywords: laser; initiation; PETN; nanomaterials; explosion; a light-detonator; aluminium.

One is a perspective way development of new energy materials for detonators initiated by laser impulses is investigation of mixed compositions of the secondary explosives and nanosized energy-intensive particles. As an initiation source laser on phosphate glass with neodymium was used (1060 nm, 20 ns). Into PETN powder nanoparticles Al (120 nm) were added up to needed concentration. Explosion probability subject to energy density of laser impulses was measured and critical energy $W_{0.5}$ was measured. Its value corresponds to 50% of explosion probability for samples with characteristic particle size 100-120 nm and with various Al content made by gaseous phase synthesis. It is discovered during experiment sensibility to the laser influence can be regulated in a wide range. Optimal nanoparticle concentration under which maximum sensibility $W_{0.5} = 1.4 \pm 0.1$ J/cm^2 is achieved is 0.1%. Thus sensibility to the laser impact increasing is 100 during this experiment. In the frame of MI theory coefficients of absorption effectiveness of aluminum impurities in PETN matrix are calculated. It is showed maximum value of effective coefficient is obtained when impurity radius is R 100 nm. All these results permit to propose in the field of laser emission nanoparticles are heated up to very high temperatures and “hot points” appear which are sites of chemical decomposition in a sample matrix, so it is resulted in explosion.

PETN monocrystals detonation under electron-beam initiation

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Keywords: PETN; electron beam; products of PETN detonation.

Space-dynamic characteristics of PETN glow under electron pulsed beam exposure and glow spectrum of detonation products are studied. Investigated objects are PETN monocrystals with 1.1÷1.8 mm thickness and cross size 3÷5 mm. Electron beam charac-teristics are effective electron energy 0.25 MeV, pulse length 20 ns, energy density up to 40 J/sm2. During ionization impulse radioluminescence and glow are observed, the latter spreads from irradiated sample surface in vacuum with rate 5000-6500 m/s for various samples. Electron beam absorption in a crystal irradiated layer is resulted in forming and spreading of a shock wave. In the time of shock reflection from a barrier on the sample back side, which has more acoustic hardness than PETN monocrystal, there is strengthen-ing of a shock. All this is resulted in detonation which is observed as glow spreading from back side to irradiated one with a rate 7500-8500 m/s for various samples. Glow spec-trums of scattering products were measured in interval 400-700 nm. It is discovered dur-ing action of electron impulse glow appears and it has spectrum similar to radiolumines-cence one and it is connected with surface dispersion under action of high-current electron beam .Spectrum of scattering products of PETN detonation is a broad glow band growing in IR-area. Lines which impose over total spectrum are identified as nitrogen molecular glow. Observed glow is short-wave recession of glow band with maximum is 1.5 eV. Glow spectrum is not described by Plank formula so it has luminescence origin. In the presence time there is no simple interpretation of this luminescence We suppose this glow is con-nected with excited NO3 molecules.

The thermal decomposition of 1,3-diphenyltriazen

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Keywords: thermal decomposition; 1,3-diphenyltriazen.

The thermal decomposition kinetics of 1,3-difeniltriazena has been studied by a manometrical method in solid and liquid conditions, and in a solution in m-DNB. In a solution and in liquid the reaction rate is described by the equation of the first order. Full gas evolution makes 120 sm^3/g.

Parameters of the equation of Arreniusa in m-DNB are equal: Eact = 36,2±1,5 kcal/mol, lgA = 16±0,5 c-1, in rasplave Eact=39,9±1,5 kcal/mol, lgA = 17,5±0,5 c-1, in a solid Eakt=38,2±2,5 kcal/mol, lgA = 16,1±1 c-1. At transition from a liquid state to solid rate in addition to Arrenius' temperature dependence rate of reaction of thermodecomposition decreases in the range of 100-90C in 6 times. In 1,3-difeniltriazene three reasons operate, able to reduce braking effect of a lattice: a little activation volume, a successful arrangement of the reactionary center concerning emptiness of packing and low factor of packing. However these reasons haven't rendered appreciable influence on braking effect of reaction.

Preparation and characterization of monolithic nitrocellulose-cellulose composites

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Keywords: nitrocellulose-cellulose composites; reactive armour.

Monolithic nitrocellulose-cellulose composites were prepared by separately cross-linking the mixed precursors (NC + C) with hexamethylene diisocyanate (HDI). The synthesis were optimised according to component mass ratio, HDI, solvent and catalyst concentra-tion. The concentrations of reactants and cure catalyst are the most important factors. The general method of synthesis involved dissolving HDI and catalyst in methylene chloride and next wetting a NC-C mixture with the solution. The resulting mixture was placed in a sealed box for cross-linking at a room temperature. Finally the solvent was evaporated at a temperature of ca. 40 oC. The obtained NC-C composites were characterized using TG/DTA and sensitivity to friction and drop weight impact, and used as energetic materi-als in reactive armour elements.

Ability of explosives detector dogs to generalize odor of TNT

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Keywords: dogs; explosive detection; TNT.

The use of explosive detector dogs has become quite common worldwide over the last decades. Despite enormous efforts that were invested into the research of olfaction principles there still remains lot of unanswered questions regarding olfaction and use of specially trained dogs. In our study we used explosive detector dogs (n=5) that were previously trained to detect flaked pure TNT, to see if they would be able to generalize trained odor and detect TNT of different origin and content of volatiles. Despite the fact that dogs demonstrated flawlessly their ability to detect flaked TNT they failed to respond to the TNT sample of different origin.

Synthesis and energetic properties of 5,5'-dinitrimino-3,3'-methylene-1H-1,2,4-triazole and its nitrogen rich salts

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Keywords: triazoles; methylene-bridged; nitrogen-rich salts; nitramines; crystal structure; energetic performance.

The synthesis of 5,5´-dinitrimino-3,3'-methylene-1H-1,2,4-triazole (1) and selected nitrogen rich salts are presented. All compounds were fully characterized in terms of sensitivity and energetic properties. Besides a chemical characterization including multinuclear magnetic resonance study (1H, 13C, 14N) and vibrational analysis (IR, Raman), X-Ray diffraction was performed. Thermal stability was performed using differential scanning calorimetry. Detonation parameters (EXPLO5 code) were calculated based on CBS-4M computed heats of formation. The presented compounds show excellent thermal stabilities and are therefore of interest for possible applications as HEDM.

Acknowledgment

Financial support of this work by the Ludwig-Maximilian University of Munich (LMU), the U.S. Army Research Laboratory (ARL), the Armament Research, Development and Engineering Center (ARDEC), the Strategic Environmental Research and Development Program (SERDP) and the Office of Naval Research (ONR Global, title: "Synthesis and Characterization of New High Energy Dense Oxidizers (HEDO) - NICOP Effort ") under contract nos. W911NF-09-2-0018 (ARL), W911NF-09-1-0120 (ARDEC), W011NF-09-1-0056 (ARDEC) and 10 WPSEED01-002 / WP-1765 (SERDP) is gratefully acknowledged. The authors acknowledge collaborations with Dr. Mila Krupka (OZM Research, Czech Republic) in the development of new testing and evaluation methods for energetic materials and with Dr. Muhamed Sucesca (Brodarski Institute, Croatia) in the development of new computational codes to predict the detonation and propulsion parameters of novel explosives. We are indebted to and thank Drs. Betsy M. Rice and Brad Forch (ARL, Aberdeen, Proving Ground, MD) and Mr. Gary Chen (ARDEC, Picatinny Arsenal, NJ) for many helpful and inspired discussions and support of our work.

Synthesis and energetic properties of 5,5'-dinitrimino-3,3'-azo-1H-1,2,4-bistriazole - A promising RDX replacement

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Keywords: triazoles; azo-functionality; nitrogen-rich salts; nitramines; crystal structure; energetic performance.

The synthesis of 5,5´-diamino-3,3´-azo-1H-1,2,4-triazole (3) by reaction of 5 acetylamino-3-amino-1H-1,2,4-triazole (2) with potassium permanganate is described. Compound 3 is used as starting material for the synthesis of 5,5´-dinitrimino-3,3´-azo-1H-1,2,4-triazole (4), which was subsequently reacted with organic bases (ammonia, hydrazine, guanidine, aminoguanidine, triaminoguanidine) to form the corresponding nitrogen rich triazolate salts (5−9). All substances were fully characterized by IR and Raman as well as multinuclear NMR spectroscopy, mass spectrometry and differential scanning calorimetry. Selected compounds were additionally characterized by low temperature single crystal X-ray diffraction measurements. Detonation parameters (EXPLO5 code) were calculated based on CBS-4M computed heats of formation. The presented neutral compound as well as the triaminoguanidinium salt show detonation performances comparable to RDX. High thermal stabilities and low impact as well as friction sensitivities make the presented nitrogen-rich salts interesting for possible applications as insensitive HEDM.

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Financial support of this work by the Ludwig-Maximilian University of Munich (LMU), the U.S. Army Research Laboratory (ARL), the Armament Research, Development and Engineering Center (ARDEC), the Strategic Environmental Research and Development Program (SERDP) and the Office of Naval Research (ONR Global, title: "Synthesis and Characterization of New High Energy Dense Oxidizers (HEDO) - NICOP Effort ") under contract nos. W911NF-09-2-0018 (ARL), W911NF-09-1-0120 (ARDEC), W011NF-09-1-0056 (ARDEC) and 10 WPSEED01-002 / WP-1765 (SERDP) is gratefully acknowledged. The authors acknowledge collaborations with Dr. Mila Krupka (OZM Research, Czech Republic) in the development of new testing and evaluation methods for energetic materials and with Dr. Muhamed Sucesca (Brodarski Institute, Croatia) in the development of new computational codes to predict the detonation and propulsion parameters of novel explosives. We are indebted to and thank Drs. Betsy M. Rice and Brad Forch (ARL, Aberdeen, Proving Ground, MD) and Mr. Gary Chen (ARDEC, Picatinny Arsenal, NJ) for many helpful and inspired discussions and support of our work.

Synthesis and energetic properties of novel nitramino- and nitrimino azoles and corresponding nitrogen rich salts

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Keywords: triazoles; tetrazoles; nitrogen-rich salts; nitramines; nitramines; crystal structure; energetic performance.

The syntheses of 5-nitramino-3-nitro-1H-1,2,4-triazole, 1-methyl-5-nitramino-3-nitro-1,2,4-triazole, 5-amino-1-nitraminotetrazole and 5-amino-4-methyl-1-nitriminotetrazole are presented. In addition, metathesis reactions of above mentioned compounds with various nitrogen rich cations and the resulting properties are investigated. Characterization of the compounds has been performed by low temperature X-ray diffraction measurements, IR, Raman and NMR spectroscopy, partially mass spectrometry and differential scanning calorimetry. Detonation parameters (EXPLO5) were calculated based on CBS-4M computed heats of formation and X-ray densities. In addition the impact, friction and electrical spark sensitivities were explored by the BAM drophammer, friction tester and the OZM small scale electrical discharge device. The presented compounds exhibit good thermal stabilities as well as moderate sensitivity values and are therefore of interest for possible applications as HEDM.

Keywords: Triazoles; Tetrazoles; Nitrogen-rich salts; Nitramines; Nitramines; Crystal Structure; Energetic Performance

Acknowledgment

Financial support of this work by the Ludwig-Maximilian University of Munich (LMU), the U.S. Army Research Laboratory (ARL), the Armament Research, Development and Engineering Center (ARDEC), the Strategic Environmental Research and Development Program (SERDP) and the Office of Naval Research (ONR Global, title: “Synthesis and Characterization of New High Energy Dense Oxidizers (HEDO) - NICOP Effort ”) under contract nos. W911NF-09-2-0018 (ARL), W911NF-09-1-0120 (ARDEC), W011NF-09-1-0056 (ARDEC) and 10 WPSEED01-002 / WP-1765 (SERDP) is gratefully acknowledged. The authors acknowledge collaborations with Dr. Mila Krupka (OZM Research, Czech Republic) in the development of new testing and evaluation methods for energetic materials and with Dr. Muhamed Sucesca (Brodarski Institute, Croatia) in the development of new computational codes to predict the detonation and propulsion parameters of novel explosives. We are indebted to and thank Drs. Betsy M. Rice and Brad Forch (ARL, Aberdeen, Proving Ground, MD) and Mr. Gary Chen (ARDEC, Picatinny Arsenal, NJ) for many helpful and inspired discussions and support of our work.

The conformational mechanism of influence of a high pressure for speed of monomolecular chemical reaction

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Keywords: conformers; kinetics monomolecular reactions; high pressure; mathematical model.

For the first time it is considered the kinetics monomolecular reactions for the substances consisting of a set conformers. There are substances, for example, HMX, RDX which in a solution or in vapor conditions of some set conformers. It is possible to assume that under the influence of a high pressure the parity of concentration conformers changes. And as everyone conformers has individual dependence of a constant of speed on pressure change of structure of their mix leads to respective alteration of total speed of chemical reaction. In work the mathematical analysis of the constructed model is carried out. On its basis influence of a high pressure on thermal disintegration RDX and HMX is considered.

DIEPE – Detection and Identification of Explosive Precursors and Explosives

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Keywords: DIEPE; improvised explosives; explosive precursors; IEDs.

The project Detection and Identification of Explosive Precursors and Explosives (DIEPE) is focused on the detection and traceability of explosives and precursors linked to improvised explosive devices. In the part of improvised explosive devices is primarily focused on the thirteen chemical substances, which are widely available to the general public on the market, as potential precursors to home-made explosives. Availability of 13 individual precursors in the Czech Republic, specified by Standing Committee on Precursors that assists the European Commission, was evaluated and potentially producible home-made explosives were proposed.

Low sensitive HNIW

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Keywords: HNIW; crystallization; purification; sensitivity; SEM.

The aim of this study was to obtain crystals of HNIW with high purity, regular shape, without sharp edges, and relatively small particle size to improve its sensitivity to impact. New method was applied to purify the crystals and obtain low sensitive HNIW. For com-parison, different published methods were applied for the recrystallization of HNIW based on solvent-antisolvent technique. The optimum parameters affect the crystal size and shape, types of solvent and anti-solvent, rate of addition, speed of stirring as well as using ultrasound device in stead of stirrer, were used. Fourier transform infrared spectroscopy (FTIR) was used to confirm the HNIW polymorphs. Thermal stability of the samples was studied by using Differential thermal analysis technique (DTA). Qualitative analysis of the crystal size and shape was done using scanning electron microscope devise. Laser scatter-ing particle size distribution analyzer was used for the determination of the particle size distribution. Impact sensitivity was measured for all the obtained samples. The results con-firmed that the impact sensitivity of HNIW decreases by obtaining small particles with regular shape but it is still more sensitive than other nitramines. While the obtained crys-tals from the new method has small particle size, regular shape, smooth surface without crack and lower impact sensitivity than RDX and HMX.

2-nitro and 4-nitro-*N*-nitroso-*N*-ethylaniline: crystal structures and quantum chemical calculations

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Keywords: 2-nitro-*N*-nitroso-*N*-ethylaniline; 4-nitro-*N*-nitroso-*N*-ethylaniline; crystal structure; geometry optimization.

It is known that during the action of the propellant stabilizer Centralite I the decomposition products 2-nitro-N-nitroso-N-ethylaniline (1) and 4-nitro-N-nitroso-N-ethylaniline (2) are formed. Here the molecular and crystal structures of these two compounds are presented for the first time. In addition their 1H and 13C NMR spectra are presented and discussed in relation to the molecular geometry. We also report on quantum chemical calculations at the B3LYP level of theory using aug-cc-pVDZ basis sets. The energetically favored configurations will be presented and provide a better understanding of the analytical data.

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Predicting of the physico-chemical properties of nitroaromatic compounds using QSPR models

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Keywords: explosibility; nitroaromatic compounds; QSPR; DFT.

The evaluation of the explosibility of chemical substances essentially relies on the use of experimental tests according to international regulatory schemes (UN Manual of Tests and Criteria of the Recommendations on the transport of dangerous goods, regulation (EC) N°440/2008). The recent evolution of the European regulatory framework related to chemicals (REACH, CLP) implies a quantity of works incompatible with a complete systematic experimental characterization of hazardous properties (for reason of time, cost or availability of products). For example, more than 140 000 existing substances could be under concern in the registration process of REACH. Moreover, the explosive intrinsic property of a substance ranks at the top of physico-chemical hazards that may be feared from the use of a given chemical. So, the development of methods allowing the identification of this hazardous property on the basis of chemical structures is of great interest not only for existing substances but also at the R&D stage in the development of new products. For these reasons, INERIS, in collaboration with Chimie ParisTech, develops new predictive models (alternative or complementary to experimental approaches) for the evaluation of explosibility properties of hazardous substances. The development of these predictive models lies on an original method combining the statistical tools used in quantitative structure property relationship method (QSPR), i.e. multilinear regressions, principal component analyses or decision trees, with quantum chemical calculations. The proposed contribution presents such structure-property analyses for the development of models dedicated to the prediction of three properties of potentially explosive nitroaromatic compounds (heat of decomposition, impact and electric spark sensitivities) taking into account the requirements for their use within a regulatory context, including not only their statistical validations but also their chemical interpretations.

Salts of tetrazolone– low sensitivity secondary explosives

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Keywords: tetrazolone; secondary explosives; crystal structure; detonation parameters; sensitivity.

Tetrazolone (1) is formed by diazotation of 5-aminotetrazole in the presence of CuSO4. Nitrogen-rich salts such as ammonium (6), hydrazinium (7) guanidinium (2), 1ffiaminoguanidinium (3), 1,3-diaminoguanidinium (4), 1,3,5-triamino-guanidinium (5) of tetrazolone were prepared by facile deprotonation or metathesis reactions. All compounds were characterized by single crystal X-ray diffraction, vibrational spectroscopy (IR and Raman), multinuclear NMR spectroscopy, elemental analysis and DSC measurements. The heats of formation of 2–7 were calculated using the atomization method based on CBS-4M enthalpies. With these values and the experimental (X-ray) densities several detonation parameters such as the detonation pressure, velocity, energy and temperature were computed using the EXPLO5 code. In addition, the sensitivities towards impact, friction and electrical discharge were tested using the BAM drop hammer and friction tester as well as a small scale electrical discharge device.

Highly sensitive 3,5-diazidotriazole and the binary C2N9- anion

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Keywords: triazoles; primary explosives; azide.

Hydrazinium 3,5-Diazido-1,2,4-triazolate (1) was synthesized by the reaction of hydrazine (solution in THF) and 3,5-diazido-1,2,4-triazole, which was yielded by diazotation of 3,5-diaminotriazole followed by the addition of sodium azide. Compound 1 was fully characterized including X-ray diffraction, vibrational and NMR spectroscopy, mass spectrometry and elemental analysis. The detonation parameters were calculated by the EXPLO5.04 computer code using the X-ray density and theoretically obtained energy of formation. Due to its high sensitivities 1 is classified as a primary exposive.

Determination of propellants components by gas chromatography/mass spectrometry

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Keywords: explosives; analysis; extraction; gas chromatography; mass detector.

The determination of explosives, concretely components of smokeless powders and explosives mixtures is very important part of the production of explosives. Nowadays, components of propellants are determined by HPLC/UV method or classical procedures (titration or gravimetry). GC/MS method which is presented in this paper is simpler and more sensitive then HPLC/UV. The identification of substances in unknown samples by comparing measured MS/EI spectra with library spectra is next advantage of GC/MS method. A fast, sensitive and accurate GC/MS method was developed and validated for the quantification of chemical stabilizers (diphenylamine, triphenylamine, centralites and akardite II) and gelifying agents (dibuthylphthalate, trimethylcitrate and acetyltributhylcitrate) in propellants. The method consists of a Soxhlet extraction step with dichlormethane, followed by separation on a capillary column SLB-5ms (30 m x 0.25 mm x 0.25 mm). Ionization of the analytes is carried out using electron ionization. The limit of quantification of the method was 0.042 mg•mL-1 for all compounds. The accuracy ranged from 0.44 to 0.16 mg•mL-1 for diphenylamine, 0.81 to 0.20 mg•mL-1 for triphenylamine, 0.60 to 0.06 mg•mL-1 for centralite I, 1.21 to 0.01 mg•mL-1 for centralite II, 0.00 to 0.11 mg•mL-1 for akardite II, 0.38 to 0.13 mg•mL-1 for dibuthylphthalate, 1.30 to 0.01 mg•mL-1 for trimethylcitrate and 1.78 to 0.11 mg•mL-1 for acetyltributhylcitrate in the range of 0.042–0.25 mg•mL-1.

Comparative analysis of domestic and NATO standards for gunpowder chemical stability evaluation

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Keywords: gunpowder; chemical stability; standard; HPLC; microcalorimetry; HFC.

Gunpowders are thermal unstable which results in theirs chemical decomposition during storage. Because of danger of gunpowder self-ignition in stored ammunition, in Serbia and worldwide, a great attention is given to their chemical stability control. In this paper are presented NATO and domestic standards for chemical stability evaluation of smokeless gunpowders. Also, in this paper a comparative analysis is performed on domestic and NATO standards, resulting in cognition of similarities and differences, advantages and disadvantages of domestic standard in aspect of test methodology and applied methods. In experiment were used nitrocellulose gunpowders and nitrocellulose gunpowders with addition of dinitrotoluene. All gunpowder samples were examined by HPLC, microcalorimetry and HFC method.

Investigation on rate of formation of crystallisation centres of mixtures of TNT and ammonium nitrate

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Keywords: ultrasound; TNT.

Explosive charges of waste TNT in a mixture with 5.2, 16.7, 36.2% of ammonium nitrate were investigated. The rates of formation of crystallisation centres were determined from the number of meltings with and without application of ultrasonic treatment. The conclusion to be drawn is that the ultrasonic treatment of TNT leads to an increase of the rate of formation of crystallisation centres and improves its structure.

Synthesis, physico-chemical and explosive properties of amino(oxo)-dinitromethyl-1,3,5-triazines

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Keywords: mono-dinitromethyl-1,3,5-triazine; zwitter-ionic structure; insensitive explosives.

Synthesis of three mono-dinitromethyl-1,3,5-triazines containing amino-, and oxo- functionality is reported. Two compounds have zwitter-ionic structure, and the 3rd is mono-dinitromethyl-1,3,5-trazinedione. Properties of these insensitive explosives are reported and discussed.

Influence of charged and excited states on the mechanisms of hexamethylene triperoxide diamine decomposition

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Keywords: hexamethylene triperoxide diamine; charged and excited states; decomposition mechanism.

The electronic structure of a hexamethylene triperoxide diamine (HMTP) molecule in different initial states was calculated with the use of the method of density functional theory (B3LYP/6-31+G(d)). The rupture of one of its three week oxygen bonds was considered as the primary mechanism of molecule decomposition. Several initial states of the molecule were examined: the ground state, positively and negatively charged states, the lowest triplet state. The last of the mentioned states was unstable; the rupture of the dond and subsequent restructuring of the molecule took place immediately, in the process of an optimization calculation. The other states of the molecule were stable, but the bond rupture had an exothermal character in all cases. The appropriate transition states characterizing the values of energetic barriers for bond rupture were determined. The height of the barrier was successively reduced at transferring from the ground state to the positively and negatively charged states of the molecule. Results on influence of charged and excited states on the mechanisms of decomposition of dinethyle peroxide molecules were obtained too. These results had a certain similarity to the results obtained for HMTD, but the highest energetic barrier for the oxygen bond rupture was observed here in the positively charged state.

Nanostructured, amorphous and liquid energetic materials investigated by X-ray diffraction

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Keywords: X-ray diffraction; energetic materials; amorphous materials; liquids; PBX.

X-ray powder diffraction is an established tool for the investigation of crystalline energetic materials. Within this work, diffraction patterns of energetic structures between partial crystalline, nano structured and liquid are measured, including different binders as GAP and HTPB, cellulose nitrate, gels, ionic liquids, a plastic bonded explosive (PBX), paraffin and water. The measurements show quit different patterns, which may be used to characterize the amorphous substances and even distinguish different qualities of cellulose nitrate or polymerized from liquid GAP. First evaluation steps of the measured patterns include the degree of crystallinity, molecular simulation of paraffin and comparison of calculated to measured pat-terns, and the pair distribution function (pdf). The investigations show that X-ray diffraction is a powerful tool for a simultaneous investigation of crystalline and amorphous components, for instance of a PBX.

Coating of ammonium nitrate particles by slurry evaporation

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Keywords: ammonium nitrate; hygroscopic; coating.

The spherical ammonium nitrate particles with size of 50 500 micron were prepared by melt spray. To control the hygroscopic property of the ammonium nitrate(AN) particles from surrounding atmosphere, coating test of the AN particles was performed with some polymeric materials by slurry evaporation technique. The polymeric materials selected were paraffin wax, Eudragit E 100, petroleum jelly, and octadecylamine. The slurry of ammonium nitrate in dichloromethane with a coating material was vigorously stirred with 200 rpm and dichloromethane was evaporated at 70 oC. SEM photographs revealed the polymeric materials were uniformly coated. The moisture absorption rate of the ammonium nitrate particles coated was measured in a thermostat vessel tightly sealed with the relative humidity of 72%. The effectiveness of the coating as a moisture barrier on the ammonium nitrate particles was found to be in the order, paraffin wax with octadecylamine > paraffin wax > Eudragit E100 > petroleum jelly. In particular, AN coated with 0.6% of paraffin wax and octadecylamine showed that the flowing state of AN particles was very good without agglomeration.

New generation of energetic complex pentaamminecobalt(III) perchlorates

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Keywords: 4-amino-1,2,4-triazoles pentaamminecobalt(III) perchlorates; properties of energetic complex perchlorates; compatibility.

Energetic metal complexes of pentaamminecobalt(III) perchlorates with 4-amino-1,2,4-triazoles as ligands were produced by the anation reaction of aqua pentaamminecobalt(III) perchlorate with 4-amino-1,2,4-triazoles. The compatibility of 1,1-diamino-2,2-dinitroethylene (FOX-7) with the metal complex of 4-amino-1,2,4-triazole was studied.

Application of model of part of lower limb part in ballistic experiments

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Keywords: firing wounds; indirect identification method; small arm ammunition; ballistic system.

The article deals with an application of a model of part of lower limb (human thigh) in ballistic experiments focused on evaluation of wounding effects of small arms projectiles (SAP) on human body. SAP of different designs and ballistic parameters are used for the ballistic experiments. There is also shown the essential method of indirect identification applied on the physical model that substitutes a real body part of hit man in the article. Design and creation of the physical model for ballistic experiments presume the use of both real biological tissue (pig's femur) and substitute tissue (ballistic gelatine). Ways of determination of basic properties of tissues are also described in the article. Experimentally obtained properties of the target material (pig's tissue and ballistic gelatine) are compared with properties of human tissue. The ballistic experiment is focused on research into direct effects of SAP on human femur. Additional aim of the work is examination of human bone and muscle tissue substitutions and their behaviour during small arm projectile penetration; including a movement of small arms projectile after the penetration. All experimental results are compared with real wounds of human lower limb. Differences between SAP wounding effects on the physical model and real human tissues are discussed at the end of this article.

NMR evidence for oxalic acid dinitrate ester

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Keywords: propellants; mixed anhydride; oxalic acid; nitric acid; 13C NMR; 14N NMR.

Recent theoretical calculations on the mixed anhydride of oxalic and nitric acid (1) indicate that the covalent oxalic acid dinitrate ester form should be more stable than the ionic dinitronium oxalate form. [1] Here we report on reactions intended to generate compound 1. We mainly focused on the condensation of oxalyl chloride with metal nitrates. The reactions were performed at −70 °C and their course was followed by low temperature 13C and 14N NMR spectroscopy. The NMR spectra indicate the formation of the mixed anhydride 1 at low temperatures, which is further supported by quantum chemical calculations of the 13C and 14N NMR chemical shifts. The anhydride is unstable and decomposes already at low temperatures most probably via a homolytic cleavage of the O2N-O bond.

The Puzzle of Diaminofuroxan

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Keywords: quantum chemical calculations; generation of structural isomers; thermodynamic stability.

Methods of mathematical and quantum chemistry were used to study the possible reasons for failures in synthesis of diaminofuroxan. Structural isomeric forms of this compound were generated. According to results of quantum chemical calculations (HF STO 3G, DFT B3LYP 6-31G (d) and MP2 6-31G (d)), screening of the most stable forms in the gaseous phase and in water was performed. It was shown that diaminofuroxan is not the most thermodynamically stable isomer among its structural analogs.

Crystal morphology and shock sensitivity in RDX based PBXN-109

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Keywords: RDX; LSGT; sensitivity; morpholgy.

The Shock sensitivity of RDX which was produced by woolich synthesis process in based PBXN-109 was explored by LSGT. The morphology of RDX was the main factor in this research and RDX samples were produced from recrystallization process. The mean particle size of RDX samples was 300mm 340mm. The shock pressure of RDX based PBXN-109 was respectively 41.37Kbar, 43.8Kbar before RDX surface treatment and 47.68kbar and 49.54Kbar after RDX surface treatment.

Synthesis and energetic properties of 1,1,1-trinitroethane

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Keywords: trinitro compounds; silver nitroformate; 1,1,1-trinitroethane; crystal structure; energetic properties.

The reaction of silver nitroformate with iodomethane furnishes 1,1,1-trinitroethane. Silver nitroformate is prepared from selected silver salts with nitroform. Characterization includ-ing multinuclear NMR spectroscopy, vibrational analysis (IR, Raman) as well as mass spectrometry and elemental analysis was performed. The thermal stability was studied us-ing differential scanning calorimetry and the energy of formation was calculated on the CBS-4M level of theory. Furthermore, X-ray diffraction studies were performed and the crystal structure of 1,1,1-trinitroethane is presented. The syntheses of the starting materi-als are described in detail, as well. Silver nitroformate serves as a suitable transfer agent for the trinitromethyl group and 1,1,1-trinitroethane is of potential interest as high energy dense oxidizer.

The synthesis and characterization of 4,5-dinitroimidazolate salts

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Keywords: pyrotechnics; nitration; imidazoles; crystal structure.

Abstract: The syntheses of the alkali and earth alkali salts of 4,5-dinitroimidazole is reported as well as their characterization by NMR-spectroscopy, mass spectrometry and elemental analysis. The structures were determined by single crystal diffraction and the impact and friction sensitivities were measured. With the regard to their potential use as coloring agents in pyrotechnic compositions several mixtures have been investigated. Keywords: Pyrotechnics; Nitration; Imidazoles, Crystal structure.

Modified nitramines with low sensitivity

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Keywords: NTO; DNT; 2,4-dinitroimidazole; 4,5-dinitroimidazole; nitramines; crystal structure; energetic performance.

Nucleophilic substitution reactions with potassium salts of 3-nitro-1,2,4-triazol-5-one (NTO), 3,5-dinitro-1,2,4-triazole (DNT), 2,4-dinitroimidazole and 4,5-dinitroimidazole on chloromethyl nitramines were investigated. The energetic compounds were characterized by single crystal X-ray diffraction. Besides a chemical characterization including multinuclear magnetic resonance study (1H, 13C, 14N), vibrational analysis (IR, Raman), mass spectrometry and elemental analysis were performed. Thermal stability was studied using differential scanning calorimetry. Detonation parameters (EXPLO5 code) were calculated based on CBS-4M computed heats of formation. The presented compounds show detonation performances comparable to PETN. High thermal stabilities and low impact sensitivities make the presented compounds interesting for further investigations and possible applications as insensitive HEDM.

Acknowledgment

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A highly energetic compound containing a ten-nitrogen chain

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Keywords: nitrogen-rich; tetrazoles.

An azotetrazole containing a rare chain of ten connected nitrogen atoms has been prepared. The structure of this compound was confirmed by x-ray crystallography, and the physical and explosive properties of the azo compound were characterized. This compound possesses both exceedingly high explosive performances and sensitivities.

Light effects inside of block of ballistic gel during wound ballistic firing experiments

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Keywords: terminal ballistics; wound ballistics; substitute materiál; ballistic gel; temporary cavity; pdw ammunition; bullet.

The ballistic gel is utilised as a live tissue substitute material in the area of wound ballistics for firing experiments purposes. The behaviour of ballistic gel blocks is analysed after penetration by a high velocity small calibre projectile. The undesired reaction inside the block of gel occurs during collapse of the temporary cavity and consequently skews results of experiments.

The research of the explosive charge detonation in the air using numerical modelling methods

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Keywords: ANFO; FEM; LS-DYNA; AUTODYNA; detonation in the air.

Thanks to numerical tools available nowadays such as modern computers coupled with specialized programs, specialists are able to estimate the potential of an explosive to generate a shock wave and evaluate the explosive ability to work. This paper presents results obtained during measurements of detonation processes (expansion of detonation products) in the air. Cylindrical shape explosives, based on mixtures of ammonium nitrate (ANFO) were precisely analyzed. Phenomena that occur during the explosion in the air were modeled using Autodyna and LS-Dyna programs, both as 2D and 3D models. An approximate model of detonation in the air was constructed. Due to computer analysis characteristics of the pressure wave and the shape of the detonation products cloud were estimated. The results obtained by numerical simulation were verified experimentally. Computer simulations fully correspond with the processes taking place in the air during the experiments done in polygon.

Laser initiation of PETN containing light-scattering additives

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Keywords: laser; initiation; PETN; light-scattering additives.

Recently, we demonstrated that the laser initiation of pentaerythritol tetranitrate (PETN) by neodymium laser (λ = 1060 nm) is related to the resonant photoinitiation in a weak absorption band with a maximum in the region of 1020 nm and the process has a thermo-activated nature with an activation energy of E = 0.4 eV. However, the direct implementation of resonant photoinitiation in this case is limited by a small value of the absorption coefficient ($10^{\{2}$ $cm^{\{1}$). An increase in the useful absorption of initiating radiation can be achieved by increasing the path of photons in the sample. The simplest way to solving this task consists in transforming the photon trajectory from straight to broken by scattering light on the appropriate centers. We have prepared two charges, one representing pure PETN powder and the other, a mixture of the same PETN powder and powdered MgO with a grain size of 10 μm. The MgO content in the mixture was about 0.5 wt %. The charge was placed in a copper heater and heat-treated. The sample was heated to 450 K and then cooled to a temperature of initiation (T =350 K). The samples were initiated by the first harmonic (λ = 1060 nm) of a pulsed neodymium laser with a pulse duration of τ = 20 ns. The introduction of a light-scattering additive significantly increases the efficiency of laser initiation. In our experiments, the initiation threshold changed from 35 J/cm^2 for pure PETN to 10 J/cm^2 for the PETN-MgO. The obtained results are indicative of the possibility of effectively controlling the initiation threshold using light-scattering additives and show evidence for good prospects of the practical implementation of the proposed approach.

Thermal decomposition of Mannich's bases on the base of 1-methyl-3-carbamido-1,2,4-triazole

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Keywords: Mannich's bases; thermal decomposition; kinetics; correlation; ionization constant.

The thermal decomposition kinetics of Mannich's bases on the base of 1-methyl-3-carbamino-1,2,4-triazole in the solution is studied by manometric method under the static conditions with the use of chromato-mass-spectrometry. The mechanism of decomposition is established. The activation parameters are determined for the limiting stage and the correlation equations are found, which connect the rate constant with the ionization constant of the outgoing nitro compound anion. Keywords: Mannich's bases, thermal decomposition, kinetics, correlation, ionization constant

Novel synthetic methodology of 1,2,3-triazole-embedded energetic copolyacrylates by azide-alkyne click chemistry

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Keywords: click chemistry; 1,2,3-triazole-embedded polyacrylates; 3-azidopropyl acrylate.

1,2,3-Triazole-embedded energetic polyacrylates were synthesized using Cu1-catalyzed 1,3-dipolar cycloaddition of azido-polyacrylate and dinitro alkynes. (Meth)acrylate with azido groups were polymerized via controlled radical polymerization, ATRP or RAFT. 3-Azidopropyl methacrylates(AzPMA) was polymerized via ATRP or RAFT and 2,2-dinitropropyl acrylate was polymerized via RAFT with good control of polymer molecular weight. These Poly(3-azidopropyl methacrylate) or Poly(3-azidopropyl methacrylate-co-2,2-dinitropropyl acrylate) were coupled with dinitro acetylenes via a highly efficient "click" reaction to be utilized as a promising energetic binder for PBX.

Combustion of compositions with zirconium

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Keywords: solid composite propellants; zirconium; combustion rate.

Earlier it was shown that in some kinds of rocket engines Zr may be more effective ener-getic compound than Al because of higher density of Zr. The combustion of model compositions of solid composite propellants, containing Al, Zr, has been investigated. Zr percentage in compositions under consideration reached 40 %. Combustion rates and values ν were compared with similar compositions containing 18-20% Al. It was shown that at pressure from 20 till 80 atm values ν (U=b•Pν) are close to 1.0 for compositions basing on ammonium perchlorate, Al, or Zr; combustion rates for compositions with Zr are in 2-3 times higher than with Al.

Research on the effects of deterred-coating propellants on propellant charge

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Keywords: propellants; deterrent-coating propellant; propellant charge.

In order to study the effects of deterred-coating propellants on propelling charge, closed chamber test and interrupted chamber test are used to analyze the burning of mixed charge. The characteristic that the relative combustion quality ψe at the inflection point of dp/dt-ψ curve of deterred-coating propellant charge varies with the charge density is found in closed chamber tests. Reasons of the change of ψe are analyzed by result of the intercepted chamber test. From the potential equilibrium theory and the analysis of experimental data, it is indicated that the change of ψe is corresponding to the change of ψE at the potential equilibrium point of p-t curve in interior ballistic experiments of mixed charge, which will influence the interior ballistic performance.

Phenomenon of reduction of the energetic material burning rate in the electric field: the new concept

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Keywords: solid propellant microthruster; active combustion control; liquid-viscous layer; electro-chemical phenomena.

Building a cluster of small satellites should be cheaper, more robust and more versatile than building a single huge satellite. Propulsion are a key point in the miniaturization of spacecrafts because micro and nanospacecrafts would need very small and very accurate force to realize the stabilization, the pointing and the station keeping. The solid propellant microthruster based on microelectromechanical systems technology could also bring an alternative to nanosatellites propulsion needs. The lack of restart ability of the micro solid propellant thruster can be overcome by electro-thermal supporting of the temperature and electric conductivity of the liquid-viscous layer of the solid propellant. Recent experimental work, connected with study of burning of the composite solid propellants in the electric field, show that at level of pressure more than 3 MPa is observed reduction of the burning rate.For explanation of this phenomenon in the paper suggested new concept, connected with interaction of the electric field micro-structures in the burning zone. The electric field micro-structures generated in the liquid-viscous layer gives the program for formation of the cellular-pulsating micro-structures in this layer and over the burning surface of the energetic material. Excitation of the micro-structures - one of displays of fundamental relationship of energy and matter. As show the experimental data, over the burning surface there are electric field micro-structures. In accordance with suggested concept, during interaction of the electro-magnetic fields excited in the liquid-viscous layer and electro-magnetic fields of toroidal vortex micro-structures over the burning surface occurs displacement of burning zone from the burning surface. With increase of the pressure, the sizes of micro-structures in the liquid-viscous layer decrease and also the scale of vortex micro-structures over the burning surface decrease. Accordingly, with increase of the pressure the stability of the vortex micro-structures will be decreased. At destruction of the vortex micro-structures, occurs decrease of the heat flow onto the burning surface and the burning rate decrease. Actually, this phenomenon has some analogy with phenomenon of negative erosion. Considered in the paper new ignition technology with supporting of the temperature and electric conductivity of the liquid-viscous layer can be used in the solid propulsion systems of the upper stages and of the maneuvering nano/micro- satellites. These nano/micro- satellites, when employed as unacknowledged secondary payloads, can covertly rendezvous with other space assets to perform satellite inspection and other missions to disrupt, degrade, or destroy space assets.

Activation of high-sensitivity energetic materials by electrostatic discharge using ESZ KTTV testing apparatus

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Keywords: high sensitivity EM; electrostatic discharge test; activation.

Primary explosives, pyrotechnical compositions and many special substances exhibit sensitivity to energetic effects of electrostatic discharge at the level of 10–2 to 102 μJ. Therefore, specific demands are made on the construction of testing apparatus having the corresponding resolving ability. This paper both presents the solution of special testing instruments and gives results of sensitivity measurements of several types of highly sensitive compositions by means of the multi-purpose apparatus ESZ KTTV. This instrument enables sensitivity tests of common EMs as well as those being developed by means of unified methodology. Hence the obtained test data of various EMs performed with the use of ESZ KTTV in the range of 100 μJ to 100 J can mutually be compared to a certain extent.

Aluminum powder influence on ANFO detonation parameters

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Keywords: aluminized ANFO; shock wave; detonation; impulse.

ANFO are the most often used explosives in mining industry nowadays. Their advantages are: the simplicity of production, low price and practically lack of sensibility on mechanical impacts during mechanical loading to shot – holes. ANFO have also some disadvantages: lack of waterproofness and low detonation parameters which reduce their range of use to dry blasting holes in low compactness rock masses. This paper presents the results of measurements of detonation parameters for aluminized ANFO with different amount of metallic powder. The experiment included application of flaked aluminum into granulated ammonium nitrate (V) (type "EXTRA" – company YARA) with the addition of oil FLEX 401. The content of toxic products of explosion and explosive power performance of ANFO to work ability were also discussed.

Effect of whirled teak wood dust particle size to the minimal ignition temperature

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Keywords: wood dust; minimal ignition temperature.

Wood dust is perfectly flammable. Wood dust may be ignited at a certain temperature and whirling. The contribution is focused on the determination of the impact of the particle size on the minimal ignition temperature of dust clouds from teak wood (Tectona Grandis Linn). Smaller particle size has larger specific surface and the lower explosion limit decrease. The purpose of this contribution was to determine whether the particle size of teak wood dust clouds affect the minimal ignition temperature. The minimal ignition temperature was determined for fractions 71 to 90, 90 to 150 and 150 to 200 micrometers.

Kinetics of nitrocellulose decomposition in artificially aged double base propellant

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Keywords: double base propellant; kinetics; nitrocellulose decomposition.

The ageing of double base rocket propellants (DB rocket propellants), which is a consequence of chemical reactions and physical processes that take place over time, has significant effect on their relevant properties (e.g. chemical composition, viscoelastic and mechanical properties, ballistic properties, etc.). The changes of relevant properties limit the safe and reliable service life of DB rocket propellants. This is the reason why the studying of processes and consequences (or effects) of ageing is so important. One of the most important consequences of DB rocket propellant ageing is reduction of the viscoelastic and mechanical properties as the consequence of reduction of nitroglycerine (NG) content and nitrocellulose (NC) mean molecular mass. In this paper we have studied kinetics of NC decomposition in artificially aged DB propellant. The kinetic parameters are obtained following NC mean molecular mass reduction by Gel Permeation Chromatography (GPC), during artificial ageing at elevated temperatures. It has been shown that the artificial ageing of DB propellant causes significant reduction of NC mean molecular mass, where significant changes start after 60 days of ageing at 90 °C. The activation energy obtained in this way equals 145.1 kJ/mol, which corresponds to the values obtained by M. Bohn, as well as with the our unpublished results for decomposition of NC at the accelerated decomposition stage, determined from isothermal thermogravimetric experiments for nitrocellulose propellant: 138.6 kJ/mol, at $0.02<\alpha<0.25$.

Detonation of gun powder in emulsion explosive

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Keywords: detonation physics; recycle gun powder; emulsion explosive.

The great quantity of demilitarized energetic material, due to the end-of-life of munitions or the discontinuity of their use due to armament changing, demands the knowledge of recycling routes with less environmental impact than open pit burning. Among the possible alternatives, is the recycle of such materials for co-detonation with emulsion explosive. Our study reports the main features of the compositions resulting from the mixture of single and double base gun powder, ranged from 0 to 20 (%wt), with an emulsion explosive based on ammonium nitrate aqueous solution. That includes results of theoretical calculations and experimental determination of detonation velocity, the shock sensitivity using the Gap Test, and the thermal behaviour assessment using differential thermal analysis (DTA) and thermo gravimetric analysis (TGA). Both, theoretical and experimental detonation velocities have increased for the composition that includes single or double base gun powder (7.5-10%). These results are supported by the DTA/TG results that shown higher decomposition rates for compositions with gun powder than for the emulsion explosive. The compositions with double base gun powder have shown higher shock sensitivity than the basic emulsion explosive. Compositions with single based gun powder have shown no alterations in the shock sensitivity. The results of DTA/TG analysis have shown that during the heating phase, until the decomposition temperature of the single base gun powder (190 ºC), the compositions are stable and any new chemical specimen were formed due to the mixture of the gun powder with the emulsion,. The obtained results reinforce the idea that recycle of demilitarized energetic materials for co-detonation within industrial explosives is a feasible way for its valorisation and can contribute the reduction of the overall environmental impact of the demilitarization process.

Detonability of ammonium nitrate and mixtures on its base

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Keywords: improvised explosives; ammonium nitrate; detonability; failure detonation diameter.

The results of failure diameters measurements of mixtures of granular ammonium nitrate, with different quantities of aluminum powder were reported at previous NTREM seminar. The minimal critical diameter (df=21 mm) was at content of aluminum powder C =1.3-1.5%. Oxygen balance of this mixture was OB>0, though minimal critical diameter of mixtures of oxidizers with fuels usually conforms to OB=0. The critical diameter of detonation of fine-dispersed ammonium nitrate mixture with aluminum powder at zero oxygen balance was measured in this work. At dilution of this mixture with granular ammonium nitrate was found quantity of granular ammonium nitrate at that df=21 mm, thus part of granular ammonium nitrate that reacted in previous work runs was measured.

Remarkable complexity of the metal azides: structural characterisation at extreme conditions

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Keywords: metal azides; pressure; temperature; neutron diffraction; X-ray diffraction.

Metal azides [Mn+(N3)n] have been classified as energetic materials, on account of their rapid and extremely exothermic decomposition to produce large amounts of nitrogen gas. For example, the heavy metal azides AgN3 and Pb(N3)2 transition to detonation very rapidly upon mild impetus making them ideal for use as primary explosives. Meanwhile, NaN3 has been used extensively as a compact source of N2(g) in automobile air-bags and has been proposed as a source of 'high energy-density' polynitrogen species [1,2]. The structural simplicity of the metal azides has meant that they are prime candidates for theoretical studies that wish to rationalise their varied sensitivities to detonation [3]. Furthermore, these binary compounds are ideal for modelling high-energy processes, such as explosive decomposition. Under the extreme temperatures and pressures experienced during detonation, it is common for energetic materials to undergo solid-state phase transitions, thereby affecting performance and reproducibility. It is therefore essential that detailed structural information is obtained at a range of temperature and pressure conditions for this important class of materials. Such experimental information is extremely valuable to computational chemists and physicists who seek to improve the efficacy of predictive models of energetic performance (i.e. detonation velocity, sensitivity, etc). It is for this reason that we have explored, by a combination of X-ray and neutron diffraction, the effects of extreme conditions on NaN3, CsN3, TlN3, NH4N3, AgN3 and Pb(N3)2. Despite their simple nature, our studies have shown that the inorganic azides display remarkably rich polymorphism at elevated temperatures and/or pressures with significant implications for their energetic performance. All of the six compounds studied thus far undergo at least one phase transition at extreme conditions and a total of ten new polymorphs have been identified. [1] M.I. Eremets, M.Y. Popov, I.A. Trojan, V.N. Denisov, R. Boehler, and R.J. Hemley, J. Chem. Phys., 2004, 120, 10618. [2] S.M. Peiris and T.P. Russell, J. Phys. Chem. A, 2003, 107, 944. [3] M. Cartwright and J. Wilkinson, Propellants, Explos., Pyrotech., 2010, 35, 326.

Energetic derivatives of symmetrical dimethylhydrazine (SDMH)

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Keywords: hydrazines; nitrogen compounds; energetic salts; X-ray crystallography.

N,N′-Dimethylhydrazine and several of its salts with energetic anions were synthesized and fully characterized by elemental analysis, DSC, mass spectrometry, multinuclear NMR (1H, 13C and 15N) and vibrational (Raman, IR) spectroscopy. Additionally, the solid state crystal structure of the nitrate (Triclinic, P–1, a = 5.360(2) Å, b = 5.806(2) Å, c = 6.866(2) Å, α = 113.73(2)°, β = 92.44(2)° and γ = 90.08(2)°, V = 195.4(1) Å3) and perchlorate (Or-thorhombic, Pbca, a = 11.774(2) Å, b = 11.072(3) Å, c = 14.050(3) Å, $\alpha = \beta = \gamma$ = 90°, V = 1831.6(7) Å3) salts were determined. Standard tests were used to examine the sensitivity of the compounds towards impact, friction and electrostatic discharge. Lastly, the heats of formation of the compounds were calculated by means of quantum chemical calculations and used to determine the detonation parameters.

Reaction of 1,1-dimethylhydrazine with dichloromethane and energetic methathesis products

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Keywords: hydrazines; energetic compounds.

The reaction of 1,1-dimethylhydrazine with excess dichloromethane leads to the formation of the 1-(chloromethyl)-1,1-dimethylhydrazinium cation as its chloride salt ([(CH3)2N(CH2Cl)NH2]Cl, 1). 1 was subsequently reacted with a suitable silver salt to form the nitrate ([(CH3)2N(CH2Cl)NH2]NO3, 2), perchlorate ([(CH3)2N(CH2Cl)NH2]ClO4, 3) and sulphate ([(CH3)2N(CH2Cl)NH2]2SO4, 4) salts. In a subsequent reaction, 4 was reacted with barium 5,5´-azobistetrazolate pentahydrate (Ba[N4C-N=N-CN4]*5H2O) and barium dipicrate hexahydrate (Ba[(NO2)3Ph-O]2*6H2O) to form the corresponding metathesis salts [(CH3)2N(CH2Cl)NH2]2[N4C-N=N-CN4] (5) and [(CH3)2N(CH2Cl)NH2][(NO2)3Ph-O] (6). All compounds were characterized by elemental analysis, mass spectrometry, NMR (1H and 13C) and vibrational spectroscopy (infrared and Raman). Additionally, the 15N NMR spectrum of the [(CH3)2N(CH2Cl)NH2]+ cation in the nitrate salt 2 was measured in DMSO-d6 and the solid state structure of compounds 1, 3 and 4 was determined by low temperature X-ray crystallography (1: Monoclinic P21/n, a = 7.101(1) Å, b = 10.583(1) Å, c = 8.846(1) Å; β = 90.31(1)°; V = 664.8(1) Å3. 3: Triclinic P–1, a = 5.983(1) Å, b = 7.502(1) Å, c = 9.335(1) Å; α = 93.86(1)°, β = 101.21(1)°; γ = 91.13(1)°; V = 409.8(1) Å3 and 4: Monoclinic C2/c, a = 11.674(2) Å, b = 17.503(3) Å, c = 6.616(1) Å; β = 90.27(1)°; V = 1351.8(4) Å3). Lastly, the thermal properties were studied by differential scanning calorimetry.

Preliminary verification of fortification of W/O-type emulsions with demilitarized explosives based on TNT

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Keywords: Composition B; demilitarized explosives; detonation; emulsion; TNT.

The document presents a study of dependence between detonation velocities of fortified W/O emulsion explosives and the grain size of the demilitarized TNT used for this fortification. Attention has been focused on the application of ground Composition B 50/50 as an additive to W/O mixture. It has been found that the demilitarized TNT having the grain size below 100 μm could give acceptable results if added to the W/O emulsion in the amount of 50 % by wt; TNT with larger grain size necessitates simultaneous desensitizing of the final primary explosive with microballoons. A suitable additive is ground Composition B 50/50 present in the emulsion primary explosive in the amount above 30 % by wt. The presence of metal nitrates in the fortified W/O mixtures affects negatively the detonation parameters of the final explosives.

Influence of insensitive additives on usable parameters of PBX

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Keywords: PBX; NTO.

In this paper, some results of experimental studies usable parameters of Plastic Bonded Explosives containing NTO are presented. The compositions contained 95% of explosive as a mixture RDX/NTO or HMX/NTO and 5% of PTFE. The working capacity of PBX was measured by determination of intensity of blast wave. The blast wave and positive phase impulse were determined. The tests showed, that overpressure decrease with growth of the NTO content, however the decrease of impulse is smaller than the decrease overpressure blast wave. In this work, the shaped charges of typical construction which is used to perforation in oil mining were tested. The penetration capacity of steel plate by tested shaped charges was determined. Penetration of charges including mixtures of NTO-/RDX was in the 102÷117 mm range, however for NTO/HMX it was110÷125 mm.

Relationship between bond disproportionation energy and molecular electrostatic potential

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Keywords: bond dissociation energy; bond disproportionation energy; nitroaromatic compounds; molecular electrostatic potential.

Nitroaromatic energetic materials are generally characterized by their homolytic bond dissociation energies BDE(C-NO2), which describe the C-NO2 bond fission, mostly the primary fission process under thermal, impact, shock and electric spark initiation stimuli. Theoretical calculations of BDEs are substantially influenced by inadequate treatment of electron correlation. Recently the alternative method was suggested to overcome this substantial drawback – reaction energy of an isodesmic reaction RC-NO2 + SC-H → RC-H + SC-NO2 where SC-NO2 is standard nitroaromatic compound. This reaction energy is expressed as the bond disproportionation energy DISP(C-NO2), which should inherently cancel the electron correlation effect accompanying homolytic dissociation. The bond disproportionation energies DISP(C-NO2) and bond dissociation energies BDE(C-NO2) were evaluated for 30 nitroaromatic compounds at DFT B3LYP/6-311+G(d,p)//6-311+G(d,p) level with correction of ZPE energy. These characteristics were then correlated to the most positive molecular surface electrostatic potential above the aromatic ring, VS,max(ring), and to a total charge of the most reactive nitro group in a structure, Q(NO2). Results show closer correlation of DISP(C-NO2) and BDE(C-NO2) energies to the electrostatic potential than to Q(NO2) charges.

Calculated crystal structure of 4,4'-dinitro-3,3'-diazenofuroxan

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Keywords: 4,4'-dinitro-3,3'-diazenofuroxan; molecular simulations; crystal structure.

Crystal structure of 4,4'-dinitro-3,3'-diazenofuroxan (DNDAF) was solved by molecular simulation methods to predict their possible crystal structure and properties. The calcu-lated crystal structures were compared with experimentally determined crystal structure 4,4'-dinitroazofurazan (DNAF). Predic-tion of DNDAF crystal structure was solved by di-rect calculation of DNDAF crystal structure on the base of modified molecular strategies developed previously for 4,8,10,12-tetranitro-2,6-dioxa-4,8,10,12-tetraazatetracyclo [5.5.0.03,11.05.9]dodecane (TNIW). These basic properties were compared: total crys-tal energy for calculated DNDAF and for experimental and modified DNAF, description of space group, arrangement of individual molecules in the different crystal groups. Calcula-tions were done with Cerius2 and Material Studio modelling environment with using mod-ules allowing crystal structure prediction.
[1] M. Pospíšil, P. Vávra: "Crystal Structures of Energetic Materials Calculated by Molecular Simula-tions" NTREM'07 Proceedings of the 10th Seminar „New Trends in Research of Energetic Materials" Editors Jan Ottis, Miloslav Krupka, University of Pardubice, Czech Republic, April 2007, pp. 273-285, ISBN 978-80-7194-949-7.

Test of bicyclo-HMX in propellant for 9 mm calibre pistol

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Keywords: bicyclo-HMX; closed ballistic vessel; bullet velocity; maximum chamber pressure.

By ether-ethanol technology were prepared samples of nitrocellulose flake propellant with content of 5, 10 and 20 % of bicyclo-HMX. The samples were tested in closed ballistic vessel and in 9 mm Luger pistol. Higher content of bicyclo-HMX allowed the achievement of higher bullet velocity without increasing of maximum chamber pressure.

Further exploration of 5,6,7,8-tetranitro-2,3-dihydro-1,4-benzodioxine (TNBD) - a potential thermostable HEDM

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Keywords: 5,6,7,8-tetranitro-2,3-dihydro-1,4-benzodioxine; TNBD; synthesis; X-ray crystallography; DTA; spectra; HEDM.

5,6,7,8-Tetranitro-2,3-dihydro-1,4-benzodioxine (TNBD) (molecular formula =C8H4N4O10) has been described previously in 13-th NTREM Seminar and in this paper TNBD was selected for more detailed exploration. The novel method of TNBD synthesis was developed (yield=81%). The detailed structure of this compound has been investigated by X-ray crystallography. The results of differential thermal analysis (DTA) obtained with twice re-crystallized material showed onset at 247 and isoterm at 288oC. The experimental density 1,85g/cm3 of TNBD was determined by X-ray crystallography (slightly different from previously estimated 1,907g/cm3 by computer calculations). The spectral properties of TNBD (NMR, FT-IR, Raman) were explored. The main detonation properties of TNBD calculated by EXPLO 5 code (by M. Sucesca) was slightly superior in comparison to the classic HEM - tetryl (detonation velocity - 7727 m/s; detonation pressure - 278 kbar). The obtained results might suggest TNBD as a potential thermostable HEDM.

Investigation of 1-allyl-3-methylimidazolium dicyanamide as a hypergolic fuel

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Keywords: ionic liquid; hypergolic fuel; performance calculation.

The ionic liquid 1-allyl-3-methylimidazolium dicyanamide (AMIM DCA) was characterized by thermal analysis (DSC, TGA), density and rheological measurements down to -60 °C. The hypergolic reaction of AMIM DCA with nitric acid was investigated. The enthalpy of formation was calculated from the heat of combustion and the performance with nitric acid was calculated. The calculated results were compared to hypergolic agents such as monomethylhydrazine (MMH) and unsymmetrical dimethylhydrazine (UDMH). The mass specific impulse of AMIM DCA is lower than MMH and UDMH. However, the volume specific impulse of AMIM DCA outranges the traditional hypergolic fuels. With its wide range of being liquid from -94 °C up to 200 °C, it will allow an increased operational temperature range. As an ionic liquid unlike conventional molecular liquids, it has practically no vapor phase. Therefore significantly reduced environmental risk, better storage and handling properties are expected.

Plastic explosives with energetic binding systems

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Keywords: RDX; cyclonite; PETN; plastic explosives; energetic plasticiser; butyl-NENA; DNDA 5-7; silicone.

In search of interesting high performance plastic explosives formulations, the samples were prepared of plastic explosives containing RDX or PETN particles and binding systems of Butyl-NENA, DNDA 5-7 or silicone type. Out of the variants tested, Butyl-NENA-NBR based binder systems and certain silicone combinations were found to have suitable bonding properties with sufficient adhesive capacity (tackiness) to common surfaces, like at a good quality Czech Army plastic explosive PlNp10. The energy content is, however, considerably higher. The compositions prepared show better adhesive and moulding properties in comparison with composition C-4.

Formulation and Evaluation of Plastic Bonded Explosive Compositions based on HMX and TATB

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Keywords: energetic material; fluoropolymers; plastic bonded explosives; thermal properties.

The new hybrid plastic bonded explosives (PBXs) composition of TATB/HMX/Viton A has been developed to find a favorable compromise between prime properties of explosive safety and its performance. In this article, the different PBXs compositions based on HMX, TATB with Viton A used as polymeric binder were formulated and evaluated for thermal, detonation and mechanical properties were investigated. The different PBXs compositions of HMX and TATB explosives were coated with Viton A by slurry coating process method. The resultant molding powder of PBXs compositions namely TH1090, TH2080 and TH5050 obtained from this method further pressed into cylindrical shape for detonation and mechanical properties. The thermal decomposition behavior of HMX, TATB, Viton A and PBXs formulation TH1090, TH2080 and TH5050, are important aspect related to the stability, were investigated by thermal analysis techniques. The power performance all PBXs formulations including detonation velocity and detonation pressure were determined by high speed streak photography. The results of the hybrid PBXs formulations revealed that there is a favorable compromise between the extreme safety but modest detonation performance of TATB and the modest safety but excellent detonation performance of HMX.

Studies of explosive abilities of polinitrofluorenes

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Keywords: polinitrofluorenes; thermogravimetry; IR and UV spectra.

A series of 2-nitro, 2,7-dinitro, 2,4,7-trinitro- and 2,4,5,7-tetranitrofluorenes are studied by the help of thermogravimetry and spectroscopy (IR, UV). The dependence of explosive ability vs. number of nitro-groups is shown. A test of burning velocity of 2,4,5,7-tetranitrofluorene is performed. Spectral criteria of polinitrofluorenes are discussed.

Synthesis and properties of ammonium salt of 5-nitriminotetrazole

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Keywords: nitrogen-rich compounds; salts of 5-nitroiminotetrazole; explosives.

The known methods of ammonium salt of 5-nitroiminotetrazole (A5NIT) synthesis are reviewed, and the reaction path starting from easily available substrates and giving the highest yield of A5NIT was chosen to produce this compound at a laboratory scale. A5NIT was synthesized in four steps process starting from guanidine nitrate. The final product was analyzed using 1H, 13C NMR and FTIR spectroscopy. Heat of combustion in oxygen was measured with water calorimeter. Heat of combustion of A5NIT is 1679 kJ/mol, standard enthalpy of formation calculated at 298 K using Hess' law is +152 kJ/mol. Impact and friction sensitivity of A5NIT was examined. TGA and DSC results suggested that A5NIT is stable to 223 °C. Decomposition is exothermic and no solid products of decomposition were detected.

Effect of impurities on the quality of CL-20 crystals obtained by recrystallization

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Keywords: CL-20; recrystallization; purity; friction; impact sensitivity.

The growing interest in energetic causes that research are focused on materials with improved performance and safety of explosives for a wide variety of military applications. 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (HNIW) crystal, composed of nitramine group containing high oxygen content and no halogen component in the molecular formula, is high energetic material (HEMs) with the highest density (2,044g/cm3) at ε-form of structure. The performance of CL-20 in propellant and weapon systems is highly dependent upon the crystal polymorph of CL-20. The ε – polymorph is preferred because of the high energetic performance and density and lower sensitivity compared to the other polymorph. Precipitation process is a suitable technique to improve the quality of CL-20 by receiving the ε-form. However, previous studies have shown that the recrystallization process does not remove all the contamination of CL-20. It is important to apply methods of purification to improve the chemical purity of CL-20. In the presented study the effects of impurities of raw CL-20 on the process of recrystallization was investigated. The HPLC study showed that impurities that are intermediates of synthesis of CL-20 were not completely removed in precipitation. In the present paper we described purification methods that gives CL-20 samples of higher chemical purity. Samples of CL-20 crystal obtained by recrystallization from the CL-20 with different chemical purity were compared.

Using of the probit analysis for sensitivity tests - sensitivity curve and reliability

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Keywords: probit analysis; sensitivity; friction; safety; TATP; lead azide.

The sensitivity of energetic materials is usually evaluated by using a value of initiating stimulus causing the initiation with 50% probability. The better approach is to express the sensitivity in the form of a sensitivity curve. One method of sensitivity curve calculation is a probit analysis. The friction sensitivities of crystalline and dextrinated lead azide are used to explain why is the sensitivity curve better than a single point. Crossing of the obtained sensitivity curves implys the relative sensitivity of these two samples is opposite in different regions of applied friction forces. The reliability of probit analysis is demonstrated for the case of sensitivity of TATP to friction. The same sample was measured by several different operators and the resulting sensitivity curves are in a very narrow interval.

Investigation of confined explosion of layered charges

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Keywords: layered charge; RDX.

The confined explosion of an annular layered charges composed of a phegmatised hexogen (RDXph) core and an external layer consisting of aluminium powder (Al) or a mixture of ammonium perchlorate (AP) and aluminium powder was studied. Experiments were carried out in fully and partially closed structures, i.e., in the explosion chamber of 150 dm3 in volume and in the 40 m3 volume bunker with four small holes and a doorway. Charges containing about 21 g of RDXph and about 40 g of a AP/Al mixture were tested in the chamber. The RDXph core weighed about 110 or 190 g and the external layer weighed about 140 or 280 g , respectively, composed charges fired in the bunker. AP/Al mass ratios of were 25/75, and 50/50. Two types of aluminium powder were used in the mixtures. Signals of overpressure from two piezoelectric gauges located at the chamber's wall were recorded and the influence of aluminium contents and particle size on a quasi-static pressure (QSP) was studied. Moreover, the solid residues from the chamber were analyzed to determine their composition. Results from TG/DTA measurements using a TG/DTA/DSC analyzer were used. Pressure and light histories recorded in the bunker enable us to determine blast wave characteristics and time-duration of light output. The effect of a dimension of RDXph core and aluminium particle size on blast wave parameters were also investigated. For comparison, the test for RDXph and TNT charges were also carried out.

1,3,3-trinitroazetidine (TNAZ) and some of its consititutional isomers: a DFT study

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Keywords: TNAZ; detonation parameters; DFT; Kamlet-Jacobs equations.

The computational studies on 1,3,3-trinitroazetidine (TNAZ) and its constitutional isomers are carried out at UB3LYP/6-311+G(d,p) level of theory. The optimized geometries, electronic structures and some thermodynamical properties have been obtained in their ground states. Also, detonation performances were evaluated by means of the Kamlet-Jacobs equations, based on the quantum chemically calculated densities and heat of formation values. The results show that isomers of TNAZ possess the characteristic properties of energetic materials and if these stable isomers of TNAZ can be synthesized, they may be the potential candidates for the powerful energetic materials.

Investigation of detonation of watergel explosives containing polydisperse aluminum

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Keywords: watergel explosives; aluminum powders; detonation.

Water-impregnated metal-containing compositions are high-performance and safe explosive materials characterized by very low levels of mechanical and heat sensitivity. The main objective of this work is study of effect of aluminum particle size on detonation parameters for gelled water-impregnated aluminum-containing explosives (WAE). The water-gel matrix consisted of ammonium nitrate, sodium nitrate, water and polyacrilamide. Pigment grade flaked aluminum powder PAP-2 and aluminum powders of various type: ASD-4, ASD-1 and PA-3 were added to water-gel matrix. Particle size of aluminum powders in formulations varied from 5 to 150 mm. Measurements of profiles of particle velocity vs. time, u(t), for investigated compositions carried out by means of electromagnetic technique. Detonation velocity, D, measured by means of electromagnetic technique and streak camera GFR-3. The dependencies of detonation parameters on aluminum particle size, on the charge diameter and density were obtained . The critical charge diameter in glass tubes was determinated. Detonation parameters of investigated compositions were calculated by means of SD and Real computer codes.

Investigation of detonation transfer by explosion of munition in depots

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Keywords: detonation; explosive materials; shock wave; munition.

The idea of this paper derives from the occurrence of explosions at munitions depots. In order to consider such phenomena, it is approached to literary processing of sensitivity and the process of initiation of explosive materials (EM) to an external shock wave. In addition, an analysis was also used effects influence the chemical composition and technical characteristics of certain munitions that are in operational use of the Serbian Army (VS). Guided by the existing UN tests and tests of other countries, the analysis and estimates were done on possible acceptance and transmission of detonation for selected individual and packaged munitions. In conclusion are presented problems and factors that play a crucial role in the transfer of detonation.

Method of testing "pyrogenic tablets" for ignition of solid rocket fuels

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Keywords: pyrogenic tablets ignition of solid rocket.

Solid rocket fuels require special igniting devices – pyrogenic tablets – to start burning. The ignition process has very strong influence upon the subsequent operation of the rocket engine. It is therefore important to control it as accurately as possible. In the paper we present a new formulation of the method of measuring the heat produced by the pyrogenic tablets in terms of time, with temporal resolution about 1 microsecond. The method was originally developed for investigation of the atmospheric re-entry. Here it was updated to match the presently available technology.

Analysis of experimental results of solid propellants

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Keywords: solid propellants; experimental results; temperature; strain rate.

To provide a suitable constitutive model for solid propellants, a lot of fundamental experiments have to be carried out. It is particularly interesting, that general standards for conducting basic strength properties experimental tests have not yet been fully elaborated for this class of materials. Such problems as quasi-static strain range for solid propellants or shape and dimensions of simple testing specimen are still not normalized. Also, the available data concerning the basic rheological properties of solid rocket fuels is insufficient. Though, this paper is a preliminary investigation devoted to modeling of nonlinear properties of solid propellants. In this paper the influence of the Young modulus and the proof stress on various experimental temperatures and strain rates is particularly discussed.

Characterization of distribution parameters of fragment mass and number for conventional projectiles

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Keywords: natural fragmentation; mass distribution.

Assessment of parameters of high explosive (HE) projectile fragmentation process (mass distribution and number of fragments) in most of the scientific papers is generally best described using Mott (depending on dimensionality and different scaling models) and Held equations. These methods can describe distribution and number of fragments excellent, but precise data on parameters from these equations are not available in public literature. Using experimental test of natural fragmentation for several types of HE projectiles, authors tried to find the influence of several types of projectile body materials, two types of high explosive and different projectile design on range of parameters used regularly in Mott and Held laws. Obtained data can help designers with smaller experimental experience to make faster prediction of new projectile fragmentation parameters.

Calculation of enthalpy of formation of TATP and HMTD

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Keywords: TATP; HMTD; organic peroxides; enthalpy of formation; density functional theory; isodesmic reaction.

Enthalpies of formation of TATP and HMTD have been calculated by means of method of isodesmic reactions. This method shows good agreement with experimental value of enthalpies of formation of organic peroxides. We worked out one equation of isodesmic reaction for TATP and one for HMTD. Molecular structures of all reagents in isodesmic reaction have been optimaized and total energy has been calculated. B3LYP method and 6-311G**basis set have been used for optimization of molecular structure and calculation of total energy. Enthalpies of formation of all reagents in isodesmic reaction data have been taken from NIST data base.

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The End