

Abstracts of the 19th Seminar on

New Trends in Research of Energetic Materials



Pardubice, April 20–22, 2016

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

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New Trends in Research of Energetic Materials



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Preface

This NTREM seminar is a nineteen world meeting of young people, university teachers and specialists working in the fields of teaching, research, development, processing, analysing and application of all kinds of energetic materials. A history of these meetings has shown that they are not aimed only at the exchange of professional information but also at creating a likeable milieu where young specialists from different countries have the opportunity to meet and gain personal contacts.

The above mentioned main characteristics of these meetings had positive impact on increasing of international cooperation in teaching and publication activities of our students and staff. The nineteenth meeting seems to be a good time for collecting opinions from other participants regarding the influence of our meeting on their work. We would therefore welcome opinions of participants to include them in next year 20th Seminar proceedings.

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

And traditionally, I wish to thank the members of the Scientific Committee, the authors of all the seminar papers and, last but not least, you, the participants of this seminar, for its success and its influence on the continued success and growth of all future meetings at our University of young people and university teachers working in the field of teaching, research, development, processing, analysing and application of all kinds of energetic materials.

Allow me to use this opportunity for inviting you in the name of my co-workers and myself: we are looking forward to meet you at the jubilee 20th seminar in the second half of April 2017 in the Aula Magna of our University.

Pardubice, March 22nd, 2016



Svatopluk Zeman

Characterisation and modelling of the curing reaction of HTPB with isocyanate by heat flow microcalorimetry

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Keywords: HTPB-isocyanate curing; kinetic modelling of curing; microcalorimeter measurement; heat of reaction; Arrhenius parameters of HTPB curing.

Composite rocket propellants have mostly three-dimensional polyurethane elastomers as binders. One of the high performance binders is HTPB (hydroxyl terminated polybutadiene) cured with an isocyanate. It is essential for the mechanical properties of the final rocket propellant that curing has reached a high degree of conversion during the heat treatment of the initially liquid propellant mix. To assess the degree of curing is especially important, when evaluating and assessing the ageing. Therefore, one should understand the curing kinetics of the curing reaction in order to know, when residual curing during in-service time does not interfere with loss in strain capacity by ageing. A binder formulation was investigated with heat flow microcalorimetry at several temperatures in the range of 50°C to 80°C. A kinetic model based on the bimolecular reaction between OH-terminated pre-polymer and poly-isocyanate was developed, which describes the heat flow or heat generation rates dQ/dt . The so-called equivalent ratio between OH-groups and NCO-groups is considered in the model. However, the application of the model is not straightforward in spite of the basic simplicity of the model. The reason is that the reaction of second order demands the knowledge of the real start point in time of the reaction, as well as the start concentrations of the reactants. But the start time is not directly available. Start concentrations could be calculated from ingredient mix and knowing the mix volume. Further on there are many handling procedures as kneading with the isocyanate, taking out the samples from the batch, transportation of samples to the laboratory, filling of measurement cells and finally the preparation of the measurement itself. During all these steps, the reaction is already in progress and a certain conversion is achieved already up to the time from where the measured data of heat generation rate is usable for evaluation. Moreover, unknown quantities are the total heat generation Q of the mix and in principle also the heat of reaction DQR or the enthalpy of reaction DHR . Therefore, a special modelling procedure was developed to take into consideration of all these time-temperature sections with their pre-reactions with regard to the main curing reaction in the microcalorimeter. By this procedure, the heat flow curves can be at first reconstructed and then described. With measurements at several temperatures, the Arrhenius parameters are obtained and conversion curves can be established.

Challenges in testing of energetic materials

Miloslav Krupka

OZM Research

Keywords: testing; energetic materials; OPTIMEX.

Experimental determination and calculation estimation for throwing-action of HE

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Keywords: explosives; explosive performance; relative throwing ability; cylinder test; interpolation models.

Generalization of the data on the throwing ability of the test methods using devices of various geometry (the "cylinder-test", the methods of «T-20», «M-60», etc.) was carried out. The results obtained have been analyzed. On the basis of the identified linkages for the speed of throwing ability and the composition and structure of compounds, the interpolation estimated modes were constructed. The accuracy comparison of the calculation methods was carried out.

AMES test prediction by “on-the-fly” QSAR applied to high-energy molecules

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Keywords: prediction; toxicology; energetic molecules.

In collaboration with Airbus Safran Launchers Company (ASL), a research program was set up to have, in the future, optimized tools for predicting the toxicity of High-Energy Materials (HEM). The European Union has adopted a legislation named REACH about chemical to ensure a high level of protection of human health and environment and to encourage the use, in priority, of alternative research methods such as cellular tests and predictive methods. A number of in vitro and in vivo test systems have been developed to study the effects of chemicals on cells. One of the first test describe by REACH and OECD test guidelines for mutagenicity is the Ames test. Several methods can be used to predict toxicity such as Quantitative Structure Activity Relationship (QSAR). In this study, we want to compare predictions of QSAR and “on-the-fly” QSAR (OTF-QSAR). Two databases were used. The first one contains 4204 molecules of Ames test experimental data came from the Joint Research Center. The second contains 54 HEM molecules among which 5 are experimentally known from the literature for the Ames test. The two QSAR approaches were done with the 4204 molecules as the training set and two validations methods: by Leave-On-Out (LOO) on the training set and especially by the prediction of the 5 ASL known molecules. The difference for the OTF-QSAR is that the training set was a subset of the 4204 molecules selected by various degree of similarity close to the HEM database. It was found that the OTF-QSAR predictions were more accurate and increased the efficiency of predictions. For the 5 known HEM molecules, the OFT-QSAR made a good prediction for all of them whereas only 3 with the QSAR. At the end of the study, we validate the OTF-QSAR on HEM molecules.

Study of a melt-cast composition containing NTO and FOX-7

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

1,1-Diamino-2,2-dinitroethene (FOX-7) is seemed to be very useful as an ingredient in low sensitive formulations. In this paper, a melt-cast composition containing NTO, FOX-7, TNT and wax was prepared and tested. The viscosity of the melted composition was measured. Sensitivity to impact, friction, shock wave and jet impact were determined, thermal stability and ignition temperatures were established. Some detonation properties of the composition were investigated. The heat of detonation was measured using a calorimetric bomb. Detonation pressure and velocity were determined in a plate-denting test. The results of a cylinder test were used for determination of the Gurney energy, detonation pressure and energy, and an effective exponent of isentrope and the JWL equation of state of the detonation products. The initial studies indicate FOX-7 as a potential replacement of RDX in low sensitive explosives.

Thermal decomposition and combustion characteristics of 5-amino-3,4-dinitropyrazole

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Keywords: nitropyrazoles; thermal analysis; high-pressure calorimetry; kinetic analysis; combustion parameters.

Highly nitrated five-membered heterocycles (pyrazoles), polynitropyrazoles in particular, have been actively studied as promising high-energy materials. They have high density and high enthalpy of formation combined with reduced sensitivity to external stimuli. We have studied thermal decomposition of a group of nitropyrazoles i.e. 3,4-dinitropyrazole (3,4-DNP), 3,4,5-trinitropyrazole (TNP), and 5-amino-3,4-dinitropyrazole (5-ADP). For these materials kinetic analysis has been performed. For 3,4-DNP and TNP high pressure DSC was used for the first time to suppress evaporation processes. Combustion experiments revealed the 5-ADP burning rate to be higher than that of HMX and the pressure exponent to be as low as 0.5. This value does not change upon adding ammonium perchlorate (AP) to 5-ADP as a part of a binary mixture. However, the burning rate value for such mixture exceeds one for HMX/AP binary composition. Obtained experimental results prove nitropyrazoles, 5-ADP in particular, to be promising component for novel high-energy compositions.

Characterization of laser-driven flyer plates

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Keywords: laser-driven flyer plates; shock; impact; characterization; VISAR.

A laser-driven flyer plate apparatus has been constructed and characterized. The relationship between the flyer plate's composition, heat treatment, laser fluence, and its velocity has been investigated using high speed digital videography and laser interferometry. The flyer plates are generated by firing a focused ns-pulsed Nd:YAG laser through a transparent substrate to which a metal foil has been adhered. The laser pulse is absorbed by the adhesive and back side of the foil, generating a rapidly expanding plasma that ejects a section of the metal foil, approximately 1 mm in diameter. The ejected flyer plate travels through the air at high speeds, up to 1.4 km/s. Comparisons were made at various laser fluences between three different 25 μm thick foils: two Al foils with different heat treatments and one Cu foil. Results indicate that flyer plates generated from Cu foils were significantly slower than those from Al foils, and that Al foil's heat treatment (hard or annealed) had no effect on flyer plate velocities. Analysis of the flyer plate assembly after launch showed that substrate damage caused by the expanding plasma may be limiting the flyer plate's maximum velocity, as energy used to damage the substrate is not available to accelerate the flyer.

Synthesis of tetraacetylhexaazaisowurtzitane from tetraacetyldibenzylhexaazaisowurtzitane by catalytic hydrogenolysis using a continuous flow process

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Keywords: HNIW; TAIW; continuous flow.

Synthesis of TAIW by catalytic hydrogenolysis of TADBIW, a key step for the synthesis of HNIW, has been first implemented under continuous flow conditions using the commercially available H-Cube Pro reactor. Several variables (i.e. reaction temperature, flow rate, and pressure) and the stability of the system have been investigated to optimize the operating conditions. The results show that continuous flow system provides better yield than batch system. For instance, the yield is 99% at the optimized conditions, while the best yield from batch reactions is 92%. Continuous flow synthesis of TAIW has potential applications in improving the production technologies of HNIW for its many advantages over batch reactions.

Qualification of LMP-103S – an ADN-based satellite propellant

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Keywords: satellite propellant; ADN; chemical analysis.

The most commonly used monopropellant in today's satellites is hydrazine. This compound has many benefits. Its main drawback is its high toxicity. It is not only acutely toxic, but also a suspected carcinogen. The demands on the protective measures in all handling of hydrazine – especially so in the fuelling of a satellite, where protective gear similar to a space suit must be worn – makes it increasingly expensive to use. It is listed as a substance of very high concern according to the REACH legislation. One replacement of monopropellant hydrazine is LMP-103S, which is based on ammonium dinitramide (ADN). The other components are methanol, water, and ammonia. ADN-based monopropellants were invented in a cooperation between SSC (the Swedish Space Corporation) and FOI (the Swedish Defence Research Agency). They were further developed by ECAPS, a subsidiary to SSC. One of these propellants was LMP-103S. It has been in use in space for five years in the PRISMA mission, which is a demonstrator mission focused on formation flying and rendezvous technology in space. The PRISMA mission was developed by SSC, with support from DLR, CNES and DTU. In order to make LMP-103S qualified for upcoming European missions, a qualification under an ESA contract, with ECAPS as main contractor and FOI, EURENCO Bofors, and Swerea Kimab as sub-contractors has been initiated. This paper describes the qualification work performed by FOI with regards to development of chemical analytical methods, thermal stability, and compatibility to different construction materials used in the propulsion system.

Synthesis of (1H-tetrazol-5-yl)furoxan ammonium salts via a two-step dehydration/[3+2] cycloaddition approach

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Keywords: 1,2,5-oxadiazole 2-oxides; cyanofuroxans; [3+2] cycloaddition; (1H-tetrazol-5-yl)furoxan ammonium salts.

A general, facile, highly effective two-step protocol for direct synthesis of (1N-tetrazol-5-yl)furoxan ammonium salts with various functional substituents based on initial effective synthesis of cyanofuroxans by dehydration of furoxancarboxylic acid amides under the action of (CF₃CO)₂O/Py followed by [3+2]-cycloaddition of cyanofuroxans to ammonium azide, generated in situ from TMSN₃ and NH₄F, has been developed.

2,4,6-trinitrotoluene molecularly imprinted membranes for selective sensors

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Keywords: 2,4,6-trinitrotoluene; imprinted film; sol-gel approach; sensor.

This paper debates the results of experimental studies related to the obtaining of 2,4,6-trinitrotoluene (TNT) molecularly imprinted films, using TNT as template (TNT-MIPs) via sol-gel method. N-(2-aminoethyl)-3-aminopropyl trimethoxy silane (DAMO-T) was used as functional monomer. The TNT-MIPs are intended to be used as sensing receptors to prepare selective sensors. Atomic force microscopy (AFM) results highlighted the effect of TNT imprinting in the copolymer matrix as the surface of the imprinted layer was quite different from that of the non-imprinted layer.

Putting the squeeze on energetic co-crystals - high pressure studies of 2(CL-20):HMX and NQ:DNP

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Keywords: energetic; co-crystal; high-pressure; CL-20; HMX; nitroguanidine; dinitropyridine; RAM.

A key challenge in the field of energetic materials is their sensitivity. Efforts have been made to mitigate this through synthesis of novel molecules; however, this is generally a complex process which has had limited success. Co-crystals – multi-component crystalline materials formed of two or more neutral co-formers – have been recently investigated as a solution to this problem, offering the possibility of tuning the performance and sensitivity of an energetic material without requiring synthesis of new compounds or complex preparation. While several energetic materials have been studied under high-pressure conditions to investigate their structural behaviour, no studies of energetic co-crystals under high-pressure have been published.

To that end, two energetic co-crystal systems have been investigated under pressure using neutron powder diffraction – 2(CL-20):HMX, and nitroguanidine:2-hydroxy-3,5-dinitropyridine (NQ:DNP). The 2(CL-20):HMX co-crystal was prepared with a ResoDyn LabRAM Resonant Acoustic Mixer using a published method that approximates solvent-drop grinding. Neutron diffraction experiments were performed on the PEARL beamline at the ISIS Neutron Source in Harwell, Oxfordshire. Smooth compression was observed in this system up to 3.5 GPa, broadly in line with predictions from DFT-D calculations, and equations of state were determined from the experimental data.

The NQ:DNP co-crystal was prepared by solvothermal co-crystallisation. A potential phase transition was observed between 1.0 and 1.4 GPa. The crystal structure of this high-pressure phase is currently under investigation.

Effect of magnesium-nitrocellulose (Mg/NC) additive on the thermal behavior of Al/CuO thermite mixtures

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Keywords: Al/CuO thermite system; Mg/NC additive; TG/DSC techniques; ignition temperature; heat of reaction.

Aluminum and a variety of metal oxides such as CuO, WO₃, MoO₃, Bi₂O₃ and Fe₂O₃ traditionally are used in thermite mixtures. Among them, the 2Al+3CuO thermite system, is particularly attractive for its low adiabatic temperature (i.e. 2570 °C), which is sufficient to vaporize a part of the copper metal formed by the reduction of the oxide. In this study, influence of magnesium-nitrocellulose (Mg/NC) additive on the thermal behavior of Al/CuO system was verified by thermogravimetry (TG) and differential scanning calorimetry (DSC) techniques. Thermite reactions are difficult to start as they require very high temperatures for ignition, e.g. for micron-Al/nano-CuO thermite, there was no reaction until 1000 °C. It was found that the ignition temperature is significantly reduced when the binary Mg/NC system is added to Al/CuO thermite system. Thermal analysis results indicated that the ignition temperature and heat of reaction of the micron-Al/nano-CuO/Mg/NC (17.5:67.5:10:5 wt.%) system reached to 630.7°C and 835.5 Jg⁻¹, respectively. Also, effect of Mg/NC additive on the thermal properties of the nano-Al/nano-CuO thermite system was investigated. According to the experimental results, by adding Mg/NC to the nano-thermite mixture (nano-Al/nano-CuO), the heat of reaction was increased considerably and upward from 478.8 Jg⁻¹ to 1893.2 Jg⁻¹.

Energetic trinitro and fluoro-dinitro ethyl ethers of 1,2,4,5-tetrazine

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Keywords: fluorodinitroethyl; hypofluorous acid; 1,2,4,5-tetrazine; N-Oxide; energetic materials.

Several new energetic ethyl ethers of 1,2,4,5-tetrazine have been synthesized. These molecules display good thermal stability and high densities. Included in our studies are a 2,2,2-trinitroethoxy 1,2,4,5-tetrazine and two dinitro-fluoroethoxy 1,2,4,5-tetrazines. One of these compounds was converted to the di-N-oxide derivative. The sensitivity of these materials towards destructive stimuli was determined, and overall the materials show promising energetic performance properties.

The effects of HMX@TATB core-shell composites on the mechanical properties of PBX

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Keywords: PBX; HMX@TATB core-shell composites; interface; mechanical property.

The mechanical property which will directly affect the structural integrity of explosive charge under complex environment is one of the most important properties of polymer bonded explosive (PBX). Studies have shown that interface debonding is the main causes of fracture in charge, because interface debonding is more likely to happen compared with the crystal fracturing even in the PBX with many initial suppression damage in crystal. In order to enhance the mechanical strength, interaction between explosive crystal and binder need to be improved firstly. As well known that adhesion work is decided by adhesion force per unit area and area. In this paper, a novel structure build with HMX@TATB core-shell composites was used to increase the interface area in PBX. The appearance of explosives was tested by scanning electron microscope (SEM) and polarizing optical microscope (POM), the quasi-static mechanical properties were tested by material testing machine, the dynamic mechanical property was tested by Split Hopkinson Pressure Bar (SHPB), and the creep resistance was tested by dynamic mechanical analysis (DMA). The results indicate that nano-sized TATB coated on micro-sized HMX result in significant change on surface morphology of HMX and the interface adhesion state between particles and polymer binder. HMX@TATB core-shell composites present rough surface and the binder embed in the surface of HMX@TATB core-shell composites. Compared to PBX-PT, the HMX@TATB core-shell composites in PBX-HQ improves the compression strength and tensile strength except for decreasing sensitivity. At the same time, PBX-HQ has better creep resistance. HMX@TATB core-shell composites may play an important role on the improvement of comprehensive performance of PBX.

Taming dinitramide anions within an energetic cationic metal-organic framework via simple anion exchange: a new strategy for synthesis and tunable properties of high energy materials

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Keywords: energetic materials; MOFs; anion exchange.

Energetic polynitro anions, such as dinitramide ion $[\text{N}(\text{NO}_2)_2^-]$, have attracted significant interest in the field of energetic materials due to their high densities and rich oxygen contents; however, most of them usually suffer from low stability. Conveniently stabilizing energetic polynitro anions to develop new high-energy materials as well as tuning their energetic properties still represents significant challenges. To address these challenges, we herein propose a novel strategy that energetic polynitro anions are encapsulated within energetic cationic metal-organic frameworks (MOFs). We presents $\text{N}(\text{NO}_2)_2^-$ -encapsulated within a three-dimensional (3D) energetic cationic MOF through simple anion exchange. The resultant inclusion complex exhibits a remarkable thermal stability with the onset decomposition temperature of 221 °C, which is, to our knowledge, the highest value known for all dinitramide-based compounds. In addition, it possesses good energetic properties, which can be conveniently tuned by changing the mole ratio of the starting materials. The encapsulated anion can also be released in a controlled fashion without disrupting the framework. This work may shed new insights into the stabilization, storage and release of labile energetic anions under ambient conditions, while providing a simple and convenient approach for the preparation of new energetic MOFs as well as the modulation of their energetic properties.

Unexpected thermolysis reactions for insensitive nitro-amino energetic compounds revealed by highly accurate quantum chemical calculations

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Keywords: thermal decomposition; activation barriers; quantum chemistry; FOX-7; TATB.

1,1-diamino-2,2-dinitroethylene (DADNE, FOX-7) is among the most promising high-performance insensitive energetic compounds [1-2]. Kinetics and mechanism of thermal decomposition are crucial for understanding the insensitivity and performance of this species. However, even though the thermal decomposition of DADNE under various conditions has been intensively studied experimentally and theoretically [3], there are still some contradictory assumptions concerning the initial reactions of its thermolysis. The reactions typical of nitroalkanes and nitroarenes (viz., C-NO₂ bond dissociation, nitro-nitrite, and nitro-aci-nitro isomerization) have been widely discussed as possible primary channels of thermal decomposition of the title compound. Moreover, the chemical mechanism of initiation of DADNE is often simply related to the “weakest” or “trigger” bond C-NO₂. However, the highly accurate CCSD(T)-F12 computations revealed that none of conventional reactions dominate the thermolysis of DADNE. On the contrary, we propose the two competing primary reaction channels specific for this particular nitro enamino species, which have never been discussed before. The rate-limiting step of DADNE thermolysis is the H-transfer (enamino-imino tautomerization) with a gas-phase activation barrier 48 kcal/mol followed by radical decomposition. Only a slightly higher overall activation barrier (55 kcal/mol in the gas phase) was found for the second channel comprised of intramolecular cyclization to oxazete-N-oxide, which is prone to fast subsequent molecular decomposition.

We also found the proposed decomposition mechanism to be relevant in the case of triaminotrinitrobenzene (TATB), another insensitive high-energy compound widely used in applications. The activation barriers of the two above discussed decomposition pathways and nitro-nitrite rearrangement are very close to each other (62 kcal/mol).

[1] Latypov, N.V.; Bergman, J.; Langlet, A. et al. *Tetrahedron*, 54 (1998) 11525. [2] Jalovy, Z.; Ek, S.; Ottis, J. et al. *J. Energ. Mat.*, 31 (2013) 87. [3] Kuklja M.M. *Adv. Quant. Chem.*, 69 (2014) 71.

The relationship between maximally achieved specific impulse and the acceptable combustion temperature in metal-free formulations of solid composite propellants

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Keywords: specific impulse achievable; combustion temperature acceptable.

The search for new high-energy compounds and formulations of solid composite propellants with high specific impulse I_{sp} values is associated with an increase in the combustion temperature T_c . However, the latter has not to exceed a certain value, depending on the type of engine. For example, today the maximally allowable T_c is 3800 K. To what value may raise I_{sp} , in condition that T_c does not exceed the given value $T_c(\text{limit})$. For CHNO-formulations the quantitative relationship between the maximally achieved I_{sp} and maximally acceptable $T_c(\text{limit})$ is determined. The first depends only on $T_c(\text{limit})$ and hydrogen percentage in the formulation.

Dissipative particle dynamics studies on the viscosity of molten TNT suspensions containing RDX nanoparticles

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Keywords: TNT; RDX; viscosity; DPD; theoretical mode.

Dissipative particle dynamics methods were used to investigate the viscosity of pure molten TNT and their suspensions added by different nano-scale RDX particles. The results show that, like pure molten TNT, the temperature dependence of viscosity of TNT suspensions containing RDX nanoparticles was found to be best represented by an Arrhenius-type relationship $\eta = ke^{Q/T}$, where η is the viscosity in mPa·s and T is the temperature in Kelvin. Q is the flow activation energy independent of temperature. Q is mainly dominated by the RDX nanoparticles contents and sizes, not shapes. A primary theoretical model to describe the viscosity of nano-scale suspensions of TNT/RDX is provided, which introduces the temperature effect comparing with those for micro-scale suspensions.

Self-organising of the micro/nano-structures of the reactionary zones and technologies for quantum modification of the properties and capabilities of the energetic materials

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Keywords: micro-scale combustion; reactionary zones; 3-D micro/nano-scale structures; synergetic oscillatory system; holographic resonance spectrum; micro-cymatic patterns.

In accordance with our novel micro-scale combustion concept, motivated excitation source of the 3-D micro/nano-scale physical structures in the energetic materials reactionary zones are the micro/nano-scale structures of the electromagnetic fields. According to our hypothesis each energetic material has a unique interactive holographic image of the reactionary zone which is the synergetic oscillatory system. The micro/nano-scale structures forms the fractal patterns in the reactionary zone and can be considered as a fingerprints of the holographic resonance spectrum of the reactionary zone. In the paper the possible technology of visualisation of the energetic material reactionary zone holographic image is considered. The set of the 3-D micro/nano- structures has the network organization which can be manipulated at a distance without the need for proximal electrodes. We suggest technology of scanning of the complex, multi-component unique resonance spectrum of all molecules in the reactionary zones and programmed transfer of the quantum information into the reactionary zones for excitation of the resonance spectrums of the predetermined set of molecules by means of resonance laser radiation or by use of the system of resonance electro-magnetic and acoustic fields. For example, under the influence of the system of electromagnetic or/and acoustic fields the random 3-D micro/nano- structures can turn into astonishing forms. Such oscillatory structures can form the cymatic patterns, in particular, the Chladni patterns. Excitation of the resonance spectrums of the predetermined set of molecules in the reactionary zones along with re-programming of the resonance spectrum of the reactionary zones gives the possibility for control by the scale and 3-D localization of the induction and energy-releasing areas and, accordingly, allows control inter-scale interaction in the small-scale aerospace propulsion systems. Excitation of the resonance spectrums of the predetermined set of molecules in the reactionary zones allows to activate and to de-activate different physical properties. Also, such excitation of the molecules is capable to induce self-synchronization of the 3-D micro/nano-scale structures and can be used for reduction of the reactionary zones sizes and for suppression of the combustion instability. The additional technical result is connected with increase of the energy-release rate in the reactionary zones.

Slow cook-off response mechanism of TATB-HMX series formulation in iron shell

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Keywords: explosive; slow cook-off; TATB; HMX; constraint.

The slow cook-off tests were done for 6 samples of TATB/HMX series formulation in the iron shell, which thickness was 4mm and inner cavity was $\Phi 60\text{mm} \times 128\text{mm}$, after analyzing the restricting intensity of different size of the slow cook-off bomb (SCB). The test results showed that the detonation reaction occurred with the formulation without TATB while lots of small fragments formed, the explosion reaction occurred with the formulation had a small quantity of TATB while lots of big fragments formed, the burning reaction occurred with the formulation had a large quantity of TATB while no fragments formed, A good explosive mixture could be made by interfusing TATB and HMX in proportion, and its series formulation had a widely use. When high energy explosive was expected, it could be gotten by interfusing about 10%TATB into a large quantity of HMX while enhanced its cook-off performance, and when the safety was needed, it could be gotten by interfusing about 25% HMX into a large quantity of TATB while its energy was enhanced.

Investigation of confined explosions of composite and layered charges

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Keywords: thermobaric explosive; composite explosive; layered charge; confined explosion; QSP.

Thermobaric explosives (TBXs) and enhanced blast explosives (EBXs) constitute a sub-family of volumetric weapons. Recently, the future trends of EBXs and TBXs materials are composites consisting of large macroscopic particles composed of at least a binder, a reactive metal and an energetic material. In the present work, the confined explosions of cylindrical homogeneous and layered charges composed of two different types of macroscopic granular multi-components RDX-based composites were investigated. For comparison, charges consisting of simple mixtures in place of the composites, TNT and RDX phlegmatized charges were also studied. The effect of the following parameters: the structure of the macroscopic granular composite, the charge type (cylindrical pressed charge or layered charge with an RDXph core), oxygen availability (air or argon atmosphere) and the aluminium particle sizes on the QSP measured inside a 150 dm³ explosion chamber as well as on the aluminium afterburning reactions was determined. Some conclusions regarding the combustion and behaviour of aluminium particles during the confined explosion of the composite and layered charges were deduced.

Cohesive zone model parameterization by molecular dynamics

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Keywords: molecular dynamics; binder-filler interaction.

Composite rocket propellants and plastic bonded high explosives are both based on elastomeric binder matrices that contain either oxidizer particles and fuel particles or high explosives particles or both types or even all three. The components in a formulation differ widely in terms of crystallinity, thermal expansion behavior and thus mechanical properties. Therefore, composites can exhibit a combination of brittle and ductile behavior, stemming from filler and binder polymer, respectively. The binder-filler interaction is the weakest in the system, and their interface is prone to detach irreversibly, when stretched beyond a critical separation distance. In experiments, the effect of adhesion can be monitored by dynamic mechanical analysis (shape of loss factors), surface tension measurements and solution calorimetry. On a microscopic level, the cohesive zone model serves as a model for separation between surfaces to describe mechanical failure. It mimics the irreversibility of crack formation: While small loading and unloading is reversible, higher strain beyond a threshold value changes the given distance-force function for further loading cycles (local damage). Quantitative parameters for this model are hardly measureable, although they are of interest for finite element simulations to explore the material on a larger space and time scale. Here, we present the complete model of a pull-off experiment in the framework of molecular dynamics simulation. In a MD-simulation, single atoms are modeled by point masses, which interact via force-fields. It can reproduce thermodynamic and mechanical properties of multi-component systems. In an earlier contribution, the thermodynamic work of adhesion (equal to a surface tension) was presented. Now, work and force of separation of surfaces including local deformation of the surfaces is discussed. It includes irreversibility during the pull-off: As external stimulus, the interface is stressed until mechanical failure. This procedure yields higher order mechanical parameters beyond the linear elasticity model, which are input parameters for finite elements simulations: energy/force of detachment, and interaction length of entangled polymer at the interface.

Solvent suppression of ions in API mass spectrometry

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Keywords: explosives; peroxides; LC/MS.

Efforts to analyze trace levels of military and improvised explosives led to the observation that certain solvent systems severely hindered detection of the desired analyte. This effect has been observed for broad classes of compounds, for example use of as little as 2% acetonitrile in the solvent carrier for atmospheric pressure ionization mass spectrometer (MS) made certain ketones, peroxides, and esters almost undetectable. In liquid chromatography LC/MS the presence of a negative ion additives is essential to the effective detection of nitramines and nitrate esters, while it may suppress the signal of nitroarenes, such as TNT. There are many scenarios where extraction of the explosive from a matrix, e.g. from soil, is essential; thus, it is important to recognize potential issues arising in subsequent analyses.

Characterization of detonation performance and shock reactivity of PBX-materials with use of Multi-Channel Optical Analyzer MCOA-UC

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Keywords: PBX; Multi-Channel Optical Analyzer; Multi-Fiber Optical Probe.

Multi-Channel Optical Analyzer MCOA-UC was developed at University of Coimbra with the goal to provide spatially resolved real time measurements of shock fields in inert and reactive materials. Up to date, the MCOA-UC is a unique and the most advanced metrology providing the meso-scale probing of the Detonation Reaction Zone (DRZ) 3D structure of detonations at best compromise between high temporal and spatial resolution (200 ps and 50-250 μm), large amount of independent registration channels (from 64 up to 256), and design simplicity. The MCOA-UC allows for spatially-resolved simultaneous measurements of reaction light emitted from detonation front, local speed of detonation front motion, and 3D-shock field induced by the DRZ in an optical monitor. In this paper, two characteristic DRZ Performance Tests and the SDT Kinetic Rate/Reaction Radiance Test, all instrumented with the MCOA-UC are presented and discussed. New approach will be presented and discussed on characterization of shock reactivity of PBX-materials via the analysis of the reaction radiance

Synthesis and properties for benzotriazole nitrogen oxides (BTzO) and tris[1,2,4]triazolo[1,3,5]triazine derivatives

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Keywords: energetic; synthesis; performance.

Herein we first report a novel method of synthesis fused ring nitrogen-enriched compounds by intramolecular cyclization reaction. Some of them were characterized by IR, ¹H and ¹³C NMR spectroscopy. Most of them exhibit outstanding positive heat of formation (155-376 kJ/mol). Densities of these compounds fall in the range between 1.7321-1.8847 g.cm⁻³, which places them in a class of relatively dense energetic materials. Their physical properties were evaluated by Gaussian 09. and EXPLO5 6.02 calculations. Their detonation velocities and pressures were calculated to fall in the range of 6713-8441 m.s⁻¹ and 14.47-30.61 Gpa.

Application of long term stored single and double base propellants for production of pyrotechnic rocket engine

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Keywords: pyrotechnic rocket engines; single base propellants; double base propellants.

It was investigated the production of pyrotechnic rocket engines from long term stored single and double base propellants (S and DBP). The adhesive (Adh) was made from DBP, dissolved in acetone. The evaporation of solvents was investigated in room and increasing temperatures. The rates of evaporation of solvents (g/min.) were measured and were determined their maximums. The samples of paper and rocket – engine casings, from Chinese firework rocket were investigated by method for determination of unknown polymers and with infra red spectroscopy. The strength of tension of samples, made from paper – (Adh) - paper, paper – (Adh)- SBP were measured. The applied SBP were with different time of storage. The thermal characteristics of S and DBP were determined and were calculated the activation energies (Eact), orders (n) and indexes (I) of decomposition reactions. The rocket engines were made from the investigated materials and were made pyrotechnic rockets. The prices of these rockets were calculated.

Thermal decomposition and combustion of cocrystals of CL-20 and linear nitramines

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Keywords: co-crystal; CL-20; 2,4-dinitro-2,4-diazapentane; 2,4-dinitro-2,4-diazaheptane; thermal decomposition; combustion.

Co-crystallization technologies are currently being pursued for enhancing or altering the physico-chemical properties of energetic materials. In cocrystals, the components are mixed at the molecular level, thus presenting excellent models to study the combustion behaviors of mixtures. In addition, the interaction between the components in the cocrystals seriously alters the melting point of the components and perhaps may also affect their thermal decomposition. The goal of this work was to study the combustion behavior and thermal decomposition of cocrystals CL-20/2,4-dinitro-2,4-diazapentane (DNP) and CL-20/2,4-dinitro-2,4-diazaheptane (CLD-2).

Nanocomposite thermite phenomena at multiple length and time scales

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Keywords: thermites; nanocomposite; aluminium; reaction mechanism; 3D printing.

The conventional route for controlling reactivity in materials has focused primarily on the formulation, or parameters such as particle size, within the formulation. Here we look at using the architectural design of materials as an alternate method to control material reactivity. Electrophoretic deposition is used to probe the effects of film thickness on flame propagation velocity in Al/CuO thermite composites, between 10 and 150 microns. We find that thick films can yield 10x faster reaction velocities than thin films, due to their ability to trap gaseous intermediate species which evolve during the reaction. 3D printing is used to generate conductive electrodes as substrates for deposition, to examine the interactive effects between neighboring reactive materials. We find that the orientation and spacing of the architecture can yield very different behavior. In these cases, the particulate film undergoes a multiphase expansion to liberate both gases and particles. With proper design, these expansion processes can be used to direct the convection of gases and/or advection of particles to modulate the forward energy transport. The results find that the material architecture, specifically the feature size and design, gives us alternate design parameters for tailoring reactivity to deliver a desired energy release rate. This is a major benefit, considering the cost, sensitivity, or environmental concerns of many existing reactive formulations, along with the persistent need for new materials with precise energy release profiles.

Computational investigation on performance and structure of six novel furazano-[3,4-d]-pyridazine-based derivatives

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Keywords: furazano-[3,4-d]-pyridazine derivatives; heat of formation; density; detonation performance; bond dissociation energy.

Six high energy density materials of furazano-[3,4-d]-pyridazine-based derivatives were designed and first reported. Afterwards, the heats of formation (HOFs), molecular stability, energetic properties of the derivatives were explored by density functional theory (DFT) at B3LYP/6-311g (d, p) level. Results show that the title compounds possess high densities (1.832-1.997 g·cm⁻³) and good detonation performance (D 8.38-9.46 km·s⁻¹, P 31.46-42.12 GPa). In addition, the bond dissociation energy of the weakest bond (N–O bond) vary from 173.283 to 178.534 kJ·mol⁻¹). The BDEs of the designed compounds are superior to that of RDX (N–NO₂ bond, 149.654 kJ·mol⁻¹) and close to that of HMX (N–NO₂ bond, 154.905 kJ·mol⁻¹). Therefore, these compounds may be potential explosives compared with RDX (D 8.75 km·s⁻¹, P 34.70 GPa) and HMX (D 9.10 km·s⁻¹, P 39.00 GPa).

Modeling the deformation behavior and detonation wave dynamics in reactive materials

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Keywords: ignition mechanisms.

Understanding the effects of shock on reactant mixing, ignition, and propagation of reaction fronts in reactive materials is important to the advancement of their use, safety, and performance. While high-pressure shock loads are commonly used to initiate high explosives, they are also used to ignite thermite compositions, through extreme deformation and mixing, which have either powder mixture or laminate geometries. The shock typically originates from high velocity impacts or a detonation front from a donor high explosive. In the case of high explosives, once initiated, controlling their shock (detonation front) pressures and the path of propagation are often of concern for which inert materials or secondary high explosives may be used for tailoring the response. To better understand the pre-ignition mixing and post-ignition wave dynamics in energetic materials under shock loading we performed simulations using the hydrocode, ALE3D. In these simulations we considered the effects of shock direction, geometry, material density, reactant spacing, and relative inert shock wave and reaction front wave speeds. Particular attention is placed on shear at the disparate material interfaces and interactions of wave fronts with inert materials.

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Synthesis and investigation of the novel thermally stable explosive: TKX-55

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Keywords: thermally stable explosive; TKX-55; crystal structure; energetic materials.

The deficiency of ‘thermally stable’ (heat resistant) explosives with both tailored performance (detonation velocity, V_{CJ} ; detonation pressure, p_{CJ} ; heat of detonation, $\Delta E U^\circ$) and low sensitivity to friction (FS), impact (IS) and electrostatic discharge (ESD) showing at the same time low solubility in water, longevity, compatibility and a practicable synthesis is known. Synthesis of covalent compounds which contain conjugated system with attached to them explosophore groups is one of the most promising approaches in order to obtain heat resistant explosives. Moreover, inclusion into conjugated system endothermic azoles functionalities improves heat of formation of the final species. That has also impact onto detonation parameters of the explosive. This study presents the preparation and investigation of the novel thermally stable explosive TKX-55. The obtained compounds were characterized by multinuclear NMR spectroscopy, IR and Raman spectroscopy, as well as mass spectrometry and elemental analysis. Low temperature single-crystal X-ray diffraction study was also performed. The thermal stabilities were measured by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). The sensitivities were investigated using the BAM drophammer and friction tests. Impact sensitivity was correlated with the electrostatic potential calculated using the Gaussian 09 software. The sensitivity towards electrostatic discharge was determined on a small-scale ESD device (OZM). The standard molar enthalpies of formation (ΔH_f°) were calculated by the atomization method and using the standard molar enthalpies of sublimation (estimated using Trouton’s rule) based on calculated gas phase absolute molar enthalpies at 298.15 K and 1 atm with CBS-4M method using the Gaussian 09 program package. By using the ΔH_f° and the densities, detonation parameters for presented compounds were calculated using EXPLO5 V6.01 thermochemical computer code. The shock reactivity of TKX-55 was measured by applying the Small Scale Shock Reactivity Test. The utility of TKX-55 is represented by its properties (V_{CJ} , p_{CJ} , $\Delta E U^\circ$, FS, IS, ESD and temperature of decomposition) which show that TKX-55 is remarkable in comparison to HNS and PYX.

Laser sensitivity of primary explosives: Synthesis and properties of complexes with 3-Hydrazino-4-amino-1,2,4-triazole (HATr) as ligand

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Keywords: 3-Hydrazino-4-amino-1,2,4-triazole; synthesis; property; laser sensitivity primary explosives.

The paper summarizes our past studies of metal complexes with 3-hydrazino-4-amino-1,2,4-triazole (HATr) as ligand. Their structures were characterized by elemental analysis, IR spectroscopy, and single-crystal X-ray diffraction reveal that HATr may adopt either bidentate chelating style to form discrete mononuclear structure or tridentate bridging-chelating fashion to construct binuclear, one-dimensional and two-dimensional structures. The sensitivities toward mechanical, thermal, and electrical stimuli were determined. Further, the function time and the ignition energy of laser initiation of cobalt(II) and nickel(II) perchlorate complexes were measured and the influence of additives was investigated.

Formation of a fine BTF-TNT energetic cocrystal by spray drying

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Keywords: energetic cocrystal; BTF; TNT; spray drying; scale-up.

The spray drying technique was applied to effective preparation of an energetic cocrystal composed of BTF (benzotrifuroxan) and TNT (trinitrotoluene) in a 1:1 molar ratio on 10g scale . The fine BTF-TNT cocrystal was confirmed by matching the powder X-ray diffraction (PXRD) pattern of the BTF-TNT cocrystal obtained from evaporation solvent. Furthermore, the thermal property and sensitivity of fine cocrystal were presented and discussed. The fine cocrystal has an H50 of 112 cm, indicating an improved safety compared with product from evaporation solvent. Moreover, spray drying provided a fast, simple and continuous methodology for preparation and scale-up of energetic cocrystals for large scale performance tests. Keywords: Energetic cocrystal; BTF; TNT; Spray drying; scale-up.

Molecular dynamics simulations of the responses of some typical energetic materials against heating and shock

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Keywords: molecular dynamics simulation; twin crystal; dislocation defects; explosive sensitivity; hot spots.

We report the early events of a twinned HMX crystal and dislocated RDX crystals, as well as perfect ones for a comparison purpose, shocked with various velocities by molecular dynamic simulations using the ReaxFF reactive force field and the multiscale shock technique. Also, the cluster evolution at early heating stages of TATB, HMX and PETN is simulated. As results, firstly, we find that the twin enhances the shock sensitivity remarkably, in agreement with our recent experimental observation. That is, it exhibits a lower shock initiation stress, higher decomposition velocities, more temperature and stress increases under the same shock conditions, relative to the perfect crystal. In addition, we find the twinning plane is hottest and the temperature decreases in terms of the distance apart from it after shock loaded earlier, suggesting possible hot spots preferred there. Secondly, the shear dynamics of four kinds of dislocated RDX crystals are modeled, and the predicted mobility decreases in an order of (010) [001]/screw (s2), (010) [001]/edge (e2), (010) 1/2[100]/screw (s1), (010)1/2[100]/edge (e1) based on their shear stress barriers denoting the initial driving force required to activate a slip system. In view of the evolution of temperatures, pressures and reactant decay rates of the shocked perfect and dislocated RDX, we confirm that the shock sensitivity is ranked as $e2 > e1 > s2 > s1 > p$. That is, all dislocations enhance the shock sensitivity of RDX, and the edge dislocations do it evidently, while screw dislocations mildly. Finally, we find that the heated TATB, HMX and PETN are much differentiated by the size, amount, proportion and lifetime of the clusters derived from them, and their favors to cluster decrease as their oxygen balance becomes less and less negative. Besides, we think that the seeming oxygen balance-sensitivity relationship is largely and essentially attributed to the role of clustering. That is, the clusters can be formed more readily for a high explosive with more negative oxygen balance, retard its energy release, secondary and further decomposition to final products of small molecules and widen its detonation reaction zone. Furthermore, it is found the C contents in the clusters increase during the clustering, in accordance with the observed soot mainly composed of C, as a final product of detonation or deflagration. All these results provide a deep understanding on the response mechanism of energetic materials against external stimuli.

Research on output energy of micro-charge explosive driven flyer

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Keywords: lead azide; micro-charge; flyer; PDV; flyer energy.

This paper summarizes the experiment results of $\Phi 0.9 \times 0.6$ mm lead azide micro-charge driven different thickness flyer's velocity by Photonic Doppler Velocimetry (PDV), compared to the calculation result of Gurney formulation, found micro-charge driven different thickness flyer's velocity lower than the calculation, obtain the velocity-time variation curve and the energy variation with distance, provide some information available for micro-explosive train design.

Reaction of S-methyl-N-nitrothiocarbamate and its salts with hydrazine

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Keywords: S-methyl-N-nitrothiocarbamate; nitrosemicarbazide.

Reaction of S-methyl-N-nitrothiocarbamate and its salts with hydrazine has been investigated. The nucleophilic substitution reaction proceeds only with the anion of S-methyl-N-nitrothiocarbamate. Hydrazine, ammonium, potassium and sodium salts of nitrosemicarbazide was synthesized. The free nitrosemicarbazide can be readily isolated from its salt by acidification with mineral acids. Synthesis of the compounds was confirmed by elemental analysis, FTIR and UV spectroscopy.

Investigation of scaled distance influence on shockwave overpressure for plastic explosive PPE-01

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Keywords: shockwave overpressure; plastic explosive; PPE-01..

This paper investigates the influence of scaled distance on shockwave overpressure for pentrite based plastic explosive PPE-01. Series of tests were conducted in order to measure the shockwave overpressure at different distances for various small explosive charges. Shockwave overpressure was measured using piezoelectric probes. Different equations for shockwave overpressure were examined to fit the the experimental data and Sadovskiy equation $\Delta p = 1.06/Z + 4.67/Z^2 + 15.5/Z^3$ has shown good agreement with the experimental data with COD 0.98134 and average relative standard error (ARS) of 0.1927.

The properties of perspective energetic heterochain polymers - hyperbranched poly([1,2,3]-triazole-[1,3,5]-triazine)s

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Keywords: hyperbranched poly([1,2,3]-triazole-[1,3,5]-triazine)s; density; stability; sensitivity; heat of formation.

Some physico-chemical properties of hyperbranched poly([1,2,3]-triazole-[1,3,5]-triazine)s synthesized by thermal azide-alkyne cycloaddition of AB₂ and A₂B monomers were studied by DLS, DSC, TGA, SEC and other methods. Density, thermo-, photo- and hydrolytic stability, shock and friction sensitivity were determined. The thermo dynamical compatibility of polymers with various plasticizers was investigated by the micro-interference method in the temperature range from 20 to 100 oC. The phase state diagrams were plotted based on the mutual solubility of polymers with plasticizers data. The interdiffusion coefficients were found in a wide range of temperatures and solution compositions of investigated systems. Heat of monomers and polymers formation was calculated from their combustion heat, which were also defined. Superb properties of hyperbranched poly([1,2,3]-triazole-[1,3,5]-triazine)s make them ideal for the development of novel energetic materials on their base.

Compatibility assessment of thermoplastic formulations

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Keywords: formulation; compatibility; differential scanning calorimetry; thermoplastic.

Prior to the large-scale preparation of any new chemical formulation an assessment of the potential reactivity between the components must be carried out. This practice, which is common to many fields including pharmaceutical science, is particularly essential in the case of energetic formulations whose chemical incompatibility may result in an unexpected and potentially explosive decomposition. The common method used to investigate incompatibility is to heat 1:1 (w/w) formulations and evaluate the variation in their thermal stability with respect to the neat, pristine explosive. The techniques used are: differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), vacuum stability and heat flow calorimetry.

As trends in energetics move towards safer formulations the components are more commonly selected for their high thermal stability and low sensitivity to initiation.

However, recently prepared thermoplastic formulations which incorporate a thermally stable explosive, hexanitrostilbene (HNS), and a selection of high-melting-point thermoplastics produced anomalous results during their compatibility assessment leading to the suggestion that historical tests originally devised for less thermally stable materials, such as N,N',N''-trinitro-1,3,5-triazacyclohexane (RDX), may not be directly transferable to the newer generations of insensitive explosive formulations.

Thermal radiation impact of DTBP fireballs

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Keywords: organic peroxide (OP); pool fire; fireball; thermal radiation; safety distance.

The burning behaviour and thermal radiation of pool fires of organic peroxides (OP) have been studied by several authors in the past. It was shown that mass burning rates, flame temperatures and thus the Surface Emissive Power (SEP) of OP exceed to that of hydrocarbons considerably. These facts lead to further investigations of even dangerous worst case scenarios i.e. related to storage and transportation. A metal drum containing 200 l of DTBP (Di-tert-butyl peroxide) is investigated under a surrounding wood fire. Due to a higher heat flux to the substance, the mass burning rate reaches multiples of an equivalent pool fire and results in several fireballs. The analyses of thermographic camera images and radiometer measurements show higher flame lengths, higher temperatures and therefore increased thermal radiation compared to OP pool fires. The resulting greater safety distances for a DTBP fireball event are discussed.

Blast performance of gun propellants

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Keywords: detonation; blast wave; propellant; nitrocellulose; nitroglycerine.

Experimental measurements of blast wave overpressure and positive impulse are usually used for blast performance analysis of energetic materials. Such results are important to represent their damage effects. Propellants detonation and blast properties data are scarce, so experimental research was done using domestic gun propellants with nitrocellulose and nitroglycerine as main energetic components. Cylindrical charges with different propellants were considered in present study. Charges had equal length and diameter, 0.5 mm thick paper casings and were loaded with 400 g of propellant. Propellants considered had different nitroglycerine content, ranging from 0 to 40.5 mas.%, as well as different grain shape and dimensions. They were detonated using standard electric detonators and spherical booster charges with 15 g of PETN-based plastic explosive. Experimental blast wave profiles were recorded using pressure sensors 137B24A and 113B51, manufactured by PCB Piezotronics Inc. Charges and measuring sensors were placed 2 m above ground, in order to minimize effect of blast wave reflection. Experimental data was analyzed in order to obtain correlations of blast performance parameters on different properties of propellants.

Solubility of 1-methyl-4,5-dinitroimidazole in different solvents

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Keywords: solubility; 1-methyl-4,5-dinitroimidazole; laser monitoring observation technique.

The solubilities of 1-methyl-4,5-dinitroimidazole (4,5-MDNI) in water, 10% nitric acid, 30% nitric acid, 50% nitric acid and ethanol were measured. The laser monitoring observation technique was used to determine the disappearance of the solid phase in a solid + liquid mixture. All data were measured at atmospheric pressure and temperatures ranging from 293.15K to 313.15K, and the effects of solvents and temperature on solubilities of 4,5-MDNI were discussed. The solubilities were fitted with an Apelblat semi-empirical equation. The results show that the semi-empirical equation is well correlated to solubility data.

Acceleration of polymer bonded powder metal liner

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Keywords: PDV; shaped charge; Photonic Doppler Velocimetry; liner; metal acceleration.

Polymer bonded, copper powder metal flexible sheet, called “plastic-metal” by these authors, is used as a liner in linear shaped charges for cutting metals in demolition, or works in which precise cut of needed in such as oil well works. In the experiments described in this paper, this liner material is subjected to explosive acceleration, and its velocity is measured using photonic Doppler velocity technique. Due to the poor reflectivity of liner to the laser beam, several setups were explored, with different levels of success. Preliminary results indicate that use of reflective foil on the liner surface or/and an extra layer of material to keep particles together is necessary to get back enough laser reflection to be able to perform any measurements. Preliminary results suggest that it should be possible to use PDV for measurement of surface velocity.

Novel nitrogen-rich energetic macromolecules based on 3,6-dihydrazinyl-1,2,4,5-tetrazin

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Keywords: macromolecules; 1,2,4,5-tetrazine.

Nitrogen-rich energetic macromolecules were synthesized by reacting dihydrazinyl-1,2,4,5-tetrazine (DHTz) with various diisocyanates. It has been shown that polymerization or cyclization reactions could take place depending on solvent systems and reaction conditions. The formed macrocycles and polymers were comprehensively characterized by IR, NMR, high resolution MS and SEM, while the thermal stability was studied by DSC. The energetic properties of our new compounds were investigated by bomb calorimetry, along with calculations using the EXPLO-5 code. It was found that macrocycle (C-DHTZ-TM) and corresponding polymer (P-DHTZ-TM) prepared on a basis of DHTz and tetramethylene diisocyanate have larger heat of combustion than RDX, GAP and polyGLYN. The C-DHTZ-TM has comparable density and larger detonation velocity than TNT. The nitrogen content of the C-DHTZ-TM and P-DHTZ-TM is larger than 47%. The thermal stability of DHTz-based energetic macromolecules was found to be higher than currently used energetic polymers including GAP, polyNIMMO and polyGLYN. The ADN based compositions bonded by 60% (by weight) of P-DHTZ-HM and P-DHTZ-MB polymers have higher theoretical specific impulse than that bonded by polyGLYN. Therefore, our new compounds could be promising ingredients as an energetic binders or fillers. Moreover, all of the macrocycles have potential to be used as energetic gelators in gel propellants

Catalyst influence on low-calorie propellant combustion

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Keywords: propellant; combustion; catalyst action mechanism; electron probe analysis; X-ray analysis.

Previously was found that lead-copper catalysts are effective only in the presence of carbon frame on the combustion surface where substantial accumulation of catalysts is taken place. Herewith the leading burning zone is above the combustion surface. It is also known that this kind of additives are slightly affect on the low-calorie propellant burning. The reasons for this are not clear, because the possibility of formation of carbon frame on the combustion surface increases with the calorie reduction of propellant. For this kind of propellants iron and nickel catalysts are effective. Nickel-lead phthalate is also increases burning rate of the low-calorie propellant. Purpose of this work is to study the influence of copper-lead and nickel-lead phthalates and NiCO₃ as catalysts on the combustion of the low-calorie propellant Size of catalyst particles is about 5 micron. Catalytic action of additives was conducted during the combustion of propellant with Ql = 2518 kJ/kg. Various amount of catalysts was added in excess of 100% into the propellant as individual and also in aggregate with various carbon materials - carbon black and multiwall carbon nanotubes (MWCNT).

Cook-off study of AP/LiBH₄ explosive

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Keywords: cook-off; mixed explosive; AP/LiBH₄; ignition temperature; thermal stability.

As the most common oxidizer used in explosives, AP possesses high density and favorable explosive characteristics. LiBH₄ is outstanding metal hydride with almost the highest hydrogen capacity, huge reaction heat release and great potential as additive compound for energetic materials. In the research, the thermal characteristics of novel mixed explosive AP/LiBH₄ were studied by a self-designed slow cook-off setup. The self-ignition temperature and decomposition pressure for the thermal explosion of AP/LiBH₄ were measured, and the results were compared with pure AP and LiBH₄. Contrast of AP/LiBH₄ and each single component AP, LiBH₄ reveals the thermal characteristics of AP/LiBH₄ as novel mixed explosive. The ignition temperature obtained in slow cook-off test for AP/LiBH₄ is 270°C, a little higher than pure AP at 259°C. Large amount of gas is generated when LiBH₄ is added to AP. AP accelerates the decomposition of LiBH₄, and the reaction quantity is greatly improved. Thermal explosion response is mainly due to the thermal reaction of AP. This research may provide potential novel energetic system in mixed explosives.

The properties of the low density emulsion based explosives

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Keywords: low density explosives; blasting properties.

Low density explosives, due to their detonation and blasting properties are appropriate choice to be used in urban areas, at short distances from structures. By decreasing the impact share in detonation energy transferred to rock mass, the intensity of seismic influence could be reduced. The emulsion matrix based explosive mixtures, sensitized by the materials with significantly lower density have reached favourable properties determined by laboratory scale tests. Based on the laboratory test results, velocity of detonation, detonation transition and initiation sensibility measured on larger diameter samples are determined in this paper. Please fill in (or paste) your abstract here. Use about 300 words.

New family of pyrometric devices for noncontact temperature measurement of energetic materials

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Keywords: pyrometer; temperature measurement.

A new family of devices for contactless measurement of energetic materials temperature at their research, production, storage and utilization is created. In these devices the method of remote measurement of absolute radiation temperature is realized. This method of measurement is passive, that is the device registers own thermal radiation of material and doesn't make power impact on an object of measurement. Fundamental feature of these devices is use of a highly sensitive pyroelectric receiver as a sensor of infrared (thermal) radiation of the studied material. This receiver doesn't demand cooling. Devices allow to fix temperature difference up to 0.3 °S within an interval (-30 . . . + 100) °S. A special version of the device provides measurement of temperatures up to 2800 °S with 1 °S discretization. Counting time is no more than 1.0 ms. The devices have a RSS port for data transmission from pyrometer to computer or control system. Please fill in (or paste) your abstract here. Use about 300 words.

Chemical interactions in mixes haloid vinyl polymers with aluminium at impact

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Keywords: polymers; explosion-like and explosion reactions; explosive mixes; sensitivity to impact.

The new method of estimation of critical parameters for impact initiation of solid individual HE on drop-weight machine, based on thermodynamic connection between thermal energy and pressure in a deformable charge and the solution of the kinetic equation connecting local heating of HE with time of its destruction is offered. There is a good agreement of calculated and experimental results.

Investigation of self-consistent model for the gas-dynamic flow reactor in the partial oxidation of hydrocarbons

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Keywords: natural gas; partial oxidation; dynamic impulse; gas dynamics equations; numerical integration.

Oxidation of light hydrocarbons is the foundation of advanced technologies in the chemical and energy industries. Understanding the physical and chemical behavior of such a complex multi-parameter system, as mixture of hydrocarbons with an oxidant, important for the effective implementation of the conversion. In connection with it is of interest to investigate adequate mathematical model, describing the process in a wide range of temperatures, pressures, flow rates in the bulk reactor. The paper considers the model which describes in terms of one-dimensional gas-dynamic approach the steady flow of the reactants in the flow reactor. Differential equations correspond to the postulates of gas dynamics and thermodynamics, take into account detailed kinetics of chemical reactions, based on C1-C2 scheme of methane oxidation. It is essential that the system of self-consistent equations, ie, equivalent to the all laws of conservation and implicit in the derivatives for the components. Earlier in the literature when considering a one-dimensional gas dynamics one use simplified, leading to explicit normal form of equations: "freezing" of the gradient cross sectional area in the equation of motion, in the energy equation discarded input of pressure and compressibility, etc. The limiting version of the model is a plug flow reactor and one-dimensional model of reactions in the gas stream. Calculations have shown that the traditional simplicity leads in the case of the oxidation of hydrocarbons to a significant distortion of concentration and thermal fields. The model correctly reproduces the basic experimental facts: Melvin delay effects MILD-regimes and allows to study controllable modes of the partial oxidation

Energetic materials research using scanning electron microscopy

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Keywords: energetic materials; scanning electron microscopy; crystalline defects; mechanical characterization.

A key-technique for the research of energetic materials is scanning electron microscopy. In this paper several examples are given of characterization studies on energetic materials, including a solid composite propellant formulation. Results of the characterization of energetic materials using scanning electron microscopy comprise the visualization of internal defects in energetic RDX crystals and in-situ tensile tests of an AP/Al/HTPB propellant. The results show that scanning electron microscopy is a robust and flexible characterization technique in the area of energetic materials.

Oscillation of thermal oxidative degradation of intumescent systems based on ammonium polyphosphate and pentaerythritol

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Keywords: oscilation; thermoanalyses.

As a key components of intumescent systems in many cases they widely use phosphorus compounds in combination with a carbon source, nitrogen heterocycles, and other special additives. We have studied the thermogravimetric behavior of intumescent composition based on ammonium polyphosphate (APP), pentaerythritol (Per), melamine (Mel) and nanoclay (OMMT). A mixture of fillers was dispersed in polyethylene of high density (HDPE) in Brabender unit at 190 °C. On the DSC curve, recorded in the air, endothermic melting peaks of HDPE were identified (126.6 °C, $\Delta H = - 46.5 \text{ J / g}$) and PFA (322.6 °C, $\Delta H = - 20.4 \text{ J / g}$), and exothermic peak HDPE (242, 9 °C, $\Delta H = 116.1 \text{ J / g}$). Unlike the pure HDPE sample (thermal degradation temperature of the beginning of 391.7 °C) on the DSC curve of filled sample with fire retardant thermal degradation is observed around 410 °C and an exothermic peak has multiplet character (sawtooth shape of the low-temperature shoulder), i.e. we can see oscillation output of products of combustion depending on temperature. On the participation of oxygen in the air in this process show corresponding curves DSC and TGA, recorded in an argon atmosphere where thermal degradation peak is not split. These data suggest that the cause of the oscillating nature of the reaction yield is thermo-oxidative degradation of fillers. An example of the known processes is oscillating Belousov-Zhabotinsky reaction and the formation of Liesegang rings in a saturated salt solution of glycerol. However, in the latter case, oscillation occurs in time, whereas oxidative degradation process is intumescent composition at higher temperatures. Some assumptions about processes were discussed.

Impact of REACH over energetic materials: toxicological assessment of alternatives substances to dibutyl phthalate

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Keywords: REACH regulation; USEtox method; toxicological impacts.

REACH regulation is a key part of the EU novel strategy to ensure a high level of chemicals safety and a competitive chemicals industry through a system for Registration, Evaluation and Authorization of Chemicals. The authorization to produce chemicals is carried out by comparing the value of some characteristics that determine their behaviour in the environment with legal thresholds for toxicity, persistence and bioaccumulation. Therefore, if the characteristics of a substance exceed the mentioned toxicity threshold, its use can be restricted or even banned. In this situation laboratories and producers need to look for alternatives, although the evaluation of potential hazards associated with possible alternative substances may be difficult. The consequences of using alternative substances for the energetic materials production, even with lower toxicity, are unknown for the production and disposal phases. The new energetic materials can be produce in higher quantities to provide the same function of conventional substances, so the overall impact can be higher than the initial solution due to impact shifting. In order to avoid this situation a Life-Cycle Assessment of the impacts of those substances should be carry out. Therefore, the objective of this study is to demonstrate how to evaluate the toxicity impacts of the appropriate alternatives for those substances banned by REACH regulation. For that purpose, it is carried out a toxicological assessment with a Life-Cycle Impact Assessment (LCIA) method in order to calculate the toxicity impacts to ecosystems and human health. The LCIA method applied in the approach mentioned above is the USEtox that calculates the impacts based on the combination of physiochemical properties for certain environmental conditions. To demonstrate the feasibility of this method it will be presented a comparative assessment of the toxicity impacts associated with dibutyl phthalate and four alternatives in order to determine the substance with lower potential toxicity.

New approach for understanding the in-situ nitration process of EGDN synthesis

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Keywords: egdn; sulfonitric mixture; gcms in-situ analysis; reaction mechanism.

The nitration process in explosives synthesis allows understanding the formation of explosophores. Therefore, it is important to know the chemical process in both industrial and Research - Development fields either for controlling the process of the explosive synthesis, acting on the process in order to increase the yield of production or for developing new explosive molecules. Despite the earlier study of nitration process, this latter is still under speculation and theory. This work treats a novel approach to understand the nitration process of ethylene glycol for EGDN synthesis in order to avoid the subversive use of the commercial ethylene glycol and inhibit the nitration process. The approach consists firstly to identify the sulfonitric mixture composition using FTIR and Raman spectroscopy, then to follow the in-situ synthesis of EGDN with gas chromatography-mass spectroscopy (GCMS) technique, the statistical study of the chromatographic area of EGDN was performed. The FTIR and Raman results have shown that the sulfuric acid proceeds to the elimination of water molecules from the nitric acid and allows the apparition of nitronium ions, this symmetric molecule have been clearly identified by Raman method. The following of the EGDN synthesis by GC-MS has shown that this process is too fast. In fact, after 10s the first apparition of EGDN is observed nevertheless the maximum of yield is reached at 24min. After that the hydrolysis phenomenon in protonic environment is observed, this leads to the decrease of the yield. The mass spectroscopy has allowed the identification of the intermediary molecules. The combination of the obtained results has led to understand EGDN synthesis by the establishment of its reaction mechanism.

Highly energetic 1,1'-dinitramino-5,5'-bitetrazoles

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Keywords: primary explosives; nitrogen-rich; nitramines; tetrazoles; crystal structure.

The synthesis of 1,1'-dinitramino-5,5'-bitetrazole and 1,1'-dinitramino-5,5'-azobitetrazole is described. The neutral compounds are extremely sensitive and powerful energetic materials. Selected metal and nitrogen-rich salts were prepared in order to tune sensitivity and performance values. Obtained compounds were characterized using low temperature single crystal X-ray diffraction, vibrational (IR, Raman) spectroscopy, multinuclear NMR spectroscopy, mass spectrometry, elemental analysis, differential thermal analysis (DTA) and differential scanning calorimetry (DSC). The sensitivities to external stimuli (impact, friction and electrostatic discharge) were determined according to Bundesamt für Materialforschung (BAM) standard methods. The energetic performances were calculated using the EXPLO5 code and support the high energetic character of the title compounds. Heats of formation were computed by the atomization method based on CBS-4M electronic enthalpies. All compounds show sensitivities in the range of primary explosives and should only be handled with great care.

High-quality cellulose obtained from various raw materials and managing the process of its production

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Keywords: cellulose; wood celluloses; cotton; lignin; molecular and structural-chemical characteristics.

The priority in search for alternative raw materials is broader use of wood celluloses, including the relatively cheap wood cellulose of “paste board” form. However, industrial production with such raw material requires improvement of the qualitative characteristics of the cellulose in use.

The determination of flash points of TKX-50, BNFF and BNTF using standard Russian methods

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Keywords: high explosives; TKX-50; BNFF; BNTF; heat sensitivity; flash point; critical temperature of thermal explosion.

Flash point value allows us to compare the explosives on the basis of the heat sensitivity to the closed heat source. Using standard Russian methods the express-method flash point ($T_{fp}(1)$) with variable temperature of the source and 5-second delay flash point ($T_{fp}(5s)$) with constant temperature of the source for dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate (TKX-50), 3,4-bis(4-nitrofurazan-3-yl)-furoxane (BNFF) and 3,4-bis(4-nitrofurazan-3-yl)furazan (BNTF) were determined. The values of $T_{fp}(1)$ and $T_{fp}(5s)$ for TKX-50 were compared with flash points of RDX, β -HMX and ϵ -CL-20, and the values of $T_{fp}(1)$ and $T_{fp}(5s)$ for BNFF and BNTF were compared with flash points of benzotrifuroxane (BTF) and high performance melt-castable explosive - 2',2',2'-trinitroethyl-4,4,4-trinitrobutyrate (TNETNB). The critical temperatures of thermal explosion for TKX-50, BNFF, BNTF, ϵ -CL-20, TNETNB were found using $T_{fp}(5s)$ values and the correlation which was found before.

Current state of cellulose nitrates production

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Keywords: cellulose nitrates; technology; plant; centrifuges.

Replacement of existing processes to remove water and alcohol dehydration is now implemented in a separate room with the help of a centrifuge of the periodic action of these procedures were combined in one device. It allowed to refuse from batch centrifuges with the involvement of manual labor. Currently working on the development of automated lines for packaging of finished products is in progress.

Analysis of primary decomposition events in nitrotetrazolatoammines of cobalt

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Keywords: quantum-chemical calculation; decomposition; complex nitrotetrazolatoamine; NCP; BNCP.

Results of quantum-chemical calculations of isolated molecules of two complex nitrotetrazolatoammines of cobalt(III) and of products of their possible primary decomposition events are presented in the paper. Such practically important complexes as (5-nitrotetrazolato-N2)pentaaminocobalt(III) perchlorate (NCP) and bis [cis (5-nitrotetrazolato-N2)]tetraaminocobalt(III) perchlorate (BNCP) were examined using quantum and common chemistry methods. Their decomposition products formed under tearing off ammonia NH₃, perchloric acid HClO₄, 5-nitrotetrazole N₄HCNO₂ molecules and nitro group NO₂ were examined too. Rather complete new results on the specified paths and energetics of decomposition were obtained. Calculations were carried out in the density functional theory approach with the use of the Gaussian 09 program set. The hybrid B3LYP functional and the 6-31+G(d) basis sets were used in calculations. A simpler basis set 3-21G was utilized for a great number of preliminary calculations of reaction decomposition paths. IR spectra were calculated for all considered initial and after decomposition molecular structures. The comparisons of obtained results with all known calculated and experimental data on the processes of decomposition of the NCP and BNCP complexes and on the spectral characteristics of the complexes and the fragments formed in the course of decomposition were made. As a more interesting result it has been shown that the most probable primary decomposition event tearing off ammonia NH₃ has several possible paths of realization.

Properties and exploding action of several explosive nitrates

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Keywords: explosive nitrite; equations of state; detonation properties; exploding action; copper barrier.

Results on physicochemical properties for six powerful explosive nitrates such as aminotetrazolium nitrate (AT-NO₃), diaminotetrazolium nitrate (DAT-NO₃), diaminouronium nitrate (DAU-NO₃), 1-amino-3-nitro-guanidinium nitrate (ANQ-NO₃), oxalylhydrazinium nitrate (OHN) and oxalylhydrazinium dinitrate (OHDN) were obtained earlier. These properties of the nitrates were determined with the use of the methods of X-ray diffraction, nuclear magnetic resonance, mass spectrometry, infrared spectroscopy, differential scanning calorimetry. Sensitivities to impact, friction and electrostatic discharge were determined too. All possible quantum-chemical properties of molecules and possible mechanisms of their decomposition were calculated in the paper using the Gaussian 09 program. The hybrid B3LYP functional and the 6-31+G(d) basis sets were used in calculations. Detonation properties of explosive nitrates and equations of state of detonation products in the form of Jones-Wilkins-Lee were calculated using the EXPLO5 V.6.02 program. These calculations were performed for explosive materials having the maximum crystalline density and for porous and having small additions of a polymeric binder ones. Comparative calculations on determination of exploding action of examined nitrates upon copper barriers were conducted in one-dimensional formulation using the ANSYS Autodyn 15 program. For comparison all similar results were obtained and presented also for such well-known and extensively used explosives as RDX and HMX.

Synthesis and evaluation of 1-alkyl-4-amino-1,2,4-triazole based energetic ionic liquid plasticizers

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Keywords: energetic ionic liquids; compatibility; plasticizers; specific impulse; energetic oxidizers; energetic binders.

Energetic ionic liquids (EILs) are receiving an increasing interest in the area of chemical propulsion due to their unique properties such as reduced vapour pressure at ambient temperatures, significantly higher densities than hydrazine, improved specific impulse, high thermal and electrical conductivity as well as high thermal stability. They are being explored for use as catalysts, monopropellants, plasticizers and also as additives in explosives and propellants. 1-R-4-amino-1,2,4-triazole (R= CH₃ and C₂H₅) with nitrate anion was synthesized from 4-amino-1,2,4-triazole by alkylation with an alkyl halide followed by an anion metathesis reaction with silver nitrate.

The synthesized compounds viz., 1-methyl-4-amino-1,2,4-triazolium nitrate (MATN) and 1-ethyl-4-amino-1,2,4-triazolium nitrate (EATN) were characterized by FT-IR. : 3432 (w), 3139 (w), 1763 (w), 1629 (w), 1572 (w), 1386 (s), 1172 (m), 1072 (w), 981 (m), 825 (m), 614 cm⁻¹ and TGA (MATN):Ti=167 deg.C and Tp = 236 deg.C. The compatibility of MATN with energetic oxidizer viz., ammonium dinitramide (ADN) and energetic binders viz., glycidylazide polymer (GAP) and polyglycidyl nitrate (PGN) were evaluated according to STANAG 4147 standard. Preliminary results show that MATN and EATN are compatible with GAP and ADN, while it showed incompatibility with PGN. The gas phase enthalpy of formation at 298.15K was computed using G2MP2 ab-initio method for the methyl and ethyl derivatives of 4-amino-1,2,4-triazole nitrates. The results showed that the compounds have positive heats of formation. MATN is stable up to 180 deg.C and decomposes in a single stage with a peak decomposition temperature of 236 deg.C assuring good stability for these at the propellant processing and curing temperatures. ADN showed a single stage decomposition in the temperature range of 180-240 deg.C, while the energetic binders GAP and PGN showed a two stage decomposition. The specific impulse, Isp of MATN (wt. % of 0 to 5) with ADN as an oxidizer and GAP and PGN as energetic binders in a non-aluminized propellant composition were calculated using NASA CEAGui at an expansion ratio of 70:1 and a chamber pressure of 70 bar assuming equilibrium flow conditions. Upon increasing the plasticizer content in a 75% solid loading of the propellant, the Isp of the propellant increases. It is shown that the Isp of the propellant with MATN plasticizer increases by 3 s and 2 s for GAP and PGN propellant respectively for a plasticizer content of 5%.

The role of the chare surface in the formation of intumescent systems

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Keywords: coke; intumescent systems.

The coke formed by heating the intumescent systems based on ammonium polyphosphate and pentaerythritol, in general, consists of three main parts: the outer surface (usually rigid with individual pores), domestic coke (loose cellular mass) and unreacted portion of intumescent layer. The presence of the latter after exposure to flame indicates the effectiveness of fire-retardant coating. The paper shows the differences in morphology and composition of the outer and inner layers of coke. On the basis of the data obtained functional properties of the outer layer is discussed. Please fill in (or paste) your abstract here. Use about 300 words.

The optimization testing of toroidal shaped charges

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Keywords: toroidal shaped charge; cutting pipes; computer simulations; Ansys AUTODYN.

The work presents the issues concerning optimization of special toroidal shaped charges, intended for cutting tubulars from inside with explosion method. The shaped charges of this type find their application in borehole mining, e.g. for cutting tubing or drill pipes in emergency and also for cutting casing pipes when a well is intended for reconstruction or liquidation. Such shaped charges are commonly used also in surface mining for liquidation of water-drain wells and multiple drainage and control systems. Examples of numerical analysis and computer simulations of functioning were presented for a charge of selected diameter (intended for cutting approx. 100 mm diameter tubulars), including several variants of its construction and conditions of use. The Ansys AUTODYN 2D software package was used in the work for optimization and simulation of toroidal shaped charges action.

Experimental study on the ammonium nitrate - based solid propellants

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Keywords: ammonium nitrate; polyurethane; pressure impulse; thermodynamic analysis; laboratory rocket motor.

This paper is related to the possibility of use the ammonium nitrate (AN) as the main propellants component, which are intended for treatments associated with the intensification of oil and gas. Various modified propellants compositions with ammonium nitrate and polyurethanes were prepared. Using laboratory rocket motor the energetic parameters (eg. maximum pressure of the gaseous products and pressure impulse) for selected propellants were determined. Furthermore, the results of thermodynamic analyzes for these propellants were performed. The influence of proposed additives on energetic parameters (i.e. impulse, calorific value, thrust coefficient) was shown. The volume of gaseous products generated per unit volume of propellant, which is important parameter in the process of hydraulic fracturing was estimated.

Highly energetic 3-trinitromethyl-5-nitramino-1H-1,2,4-triazole – synthesis and investigation

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Keywords: explosives; oxidizer; nitrogen-rich; nitramines; triazoles; crystal elucidation.

The synthesis of 3-Trinitromethyl-5-nitramino-1H-1,2,4-triazole is described. The neutral compound was obtained by nitration of 2-(5-amino-1H-1,2,4-triazol-3-yl) acetic acid and shows sensitivities in the range of primary explosives and should be handled carefully. Several nitrogen-rich salts were also synthesized in order to tune performance and sensitivities values. The obtained compounds were characterized extensively using low temperature single crystal X-ray diffraction, vibrational (IR, Raman) spectroscopy, multinuclear NMR spectroscopy, mass spectrometry, elemental analysis and differential thermal analysis (DTA). The sensitivities toward external stimuli (impact, friction and electrostatic discharge) were determined according to Bundesamt für Materialforschung (BAM) standard methods. The energetic performances were calculated using the EXPLO5 code and support the high energetic character of the title compounds. Heats of formation were computed by the atomization method based on CBS-4M electronic enthalpies.

Investigation of the effect of viton as coating agent in the presence of Mg powder on the ignition and safety properties of the Al-CuO thermite system

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Department of Chemistry

Keywords: Al/CuO thermite system; Viton; Mg powder; ignition temperature; safety properties.

In this paper, the thermal behavior of the Al/CuO thermite mixture was studied using TG-DSC at a scan rate of 20 °C min⁻¹ in an air atmosphere when viton as coating agent in the presence of Mg powder were used. Thermite reactions are difficult to start as they require very high temperatures for ignition, e.g. for micron-Al/nano-CuO thermite, there was no reaction until 1000 °C. It was found that the ignition temperature is significantly reduced when the binary Mg/Viton system is added as sensitizer. Further improvement is achieved when the Al particles are nano-sized powders. In the next step, the explosion potential (EP) was calculated for each mixture. It was found that the explosion potential is increased when the binary Mg/Viton system is added to Al/CuO mixture. The results of calculations showed that the explosion potential (EP) of the nano-Al/nano-CuO and nano-Al/nano-CuO/Mg/NC (17.5:67.5:10:5 wt. %) are - 0.66 and - 0.41, respectively.

Experimental techniques for measuring the overpressure generated by thermobaric devices

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Keywords: thermobaric; experimental technique; overpressure.

It is well known that thermo-baric explosion presents some particularities compared to condensed explosives. The main particularities between the classic explosion and aero-disperse explosion are given by the initial volume of the explosive mixture, reaction mechanism and the generated overpressure. Some thermo-baric devices have been designed. For optimization of the explosive effect it is necessary to precisely evaluate the aero-disperse explosion parameters, like generated overpressure, temperature, spatial dispersion of the fuel, etc. The time variation of overpressure in aero-disperse explosions presents some particularities compared to condensed explosions and is a key parameter for evaluation of the performances of such explosive systems. Recording the maximum generated pressure and the variation of this value in time in a precise manner is an important effort in the correct evaluation of these type of explosive systems. An acquisition system has been developed for measuring the overpressure. Although is difficult to compare the two types of phenomena, the main objective of the research effort is to evaluate the performances of the thermo-baric explosive devices in relation with the detonation of TNT, by estimating an equivalent. This can be made in two manners, either it can be compared the maximum overpressure recorded at different distances from the explosion point, either by comparison between the impetus recorded by the measurement system. The acquisition system proves to be both effective and robust enough to precisely measure the parameters of the aero-disperse explosion and to correctly evaluate the performances of a thermo-baric device by TNT equivalent.

Highly branched azide-containing poly(urethane-co-triazole)s

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Keywords: highly branched polymer; poly(urethane-co-triazole); diazidopropanol-2; diisocyanate; azide-alkyne Huisgen cycloaddition; CuAAC.

An approach to the one pot synthesis of new highly branched poly(urethane-co-triazole)s with enhanced enthalpy of formation was elaborated. It was implemented through two quantitative reactions viz. the urethane formation and the azide-alkyne Huisgen cycloaddition (AAC) or copper(I)-catalyzed azide-alkyne cycloaddition (CuAAC) reactions. The first step was the synthesis of diazide-isocyanate precursor via interaction between diazidopropanol-2 with an excess of diisocyanate (isophorone diisocyanate or hexamethylene diisocyanate). Diazide-acetylene AB₂ type monomer was obtained by one-pot reaction of the precursor with propargyl alcohol or propargyl amine on the second step. Obviously the second step reaction product may include diacetylene monomer (A₂ type) and tetraazide monomer (B₄ type), which can act during polyaddition reactions as a cross-linking or as a branching agent respectively. Due to the fact that composition of monomers may be regulated by varying the initial [NCO]/[OH] ratio and reaction conditions (solvent, catalyst, etc.), the structure of highly branched polymers received by AAC/CuAAC polyaddition can be easily controlled. A number of highly branched poly(urethane-co-triazole)s with a significant content of azide groups and triazoles were obtained and characterized by NMR, IR, DLS, DSC, TGA and SEC methods.

X-Ray studying of nitrofurazone propane carboxylic acid

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Keywords: X-ray; acid.

Studying connection represent scientific and practical interest as component of alloys that intended for creation new model injection compositions. For an establishment of interrelation between structure of substances and their behaviour in various processes at a molecular level the knowledge of a structure of researched connections is necessary, and one of objective methods of identification of a structure of new substances is the X-ray analysis. The X-ray analysis of a monocystal nitrofurazone propane carboxylic acid has been executed on automatic X-ray diffractometer Bruker Smart Apex II CCD (MoK α , graphite monochromator, λ 0.71073 Å, ω -scan) by a method of rotation. A monocystal samples for carrying out the X-ray structural analysis have been prepared from the solutions in nitromethane by the lowering temperature method. The X-ray analysis of a monocystal nitrofurazone propane carboxylic acid showed that crystals of connection C₄ H₅ N₃ O₅ monoclinic, parameters of cell at 200 S: a=6.8883(6), b=22.1267 (20), c=10.5391(10) Å, V= 1594.5(6) Å³, Z=4, symmetry space group P2(1)/n.

Comprehensive analysis of thermochemical properties for 4,4',5,5'-tetranitro-2,2'-biimidazole salts

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Keywords: Imidazoles; energetic salts; TNBI; explosives; enthalpy of formation.

Using quantum chemistry methods (DFT, CBS-4M) the structure of high-nitrogen salts of TNBI (4,4',5,5'-tetranitro-2,2'-biimidazole): (1) ammonium, (2) hydroxyl ammonium, (3a-3f) 3-amino-1,2,4-triazolium, (4) 4-amino-1,2,4-triazolium, (5) 5-aminotetrazolium, (6) semicarbazidium, (7) pyridinium, (8) pyrazolium, (9) 3-amino-pyrazolium, (10) imidazolium, (11) N-methylimidazolium, (12) 1,2,4-triazolium, (13) 3,5-diamino-1,2,4-triazolium, (14) 1,2,3-triazolium, (15) 1,5-diamino-tetrazolium, (16) 2,2'-biimidazolium has been calculated and some properties of these compounds have been estimated. The salt 2 from the series has the best explosive characteristics.

Synthesis and investigation of 3,3'-bi-(5-trifluoromethyl-1,2,4-oxadiazole) and 5,5'-bi-(2-trifluoromethyl-1,3,4-oxadiazole)

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Keywords: 1,2,4-oxadiazole; 1,3,4-oxadiazole; crystal structure; energetic materials.

The experimental and theoretical study of the closely related compounds: 3,3'-bi-(5-trifluoromethyl-1,2,4-oxadiazole) and 5,5'-bi-(2-trifluoro-methyl-1,3,4-oxadiazole) are reported. In this study they are used as model species to evaluate the suitability of the heterocyclic oxadiazole ring systems for energetic materials when the fluorine atoms in the exocyclic CF_3 groups are substituted successively by nitro groups. The title compounds were isolated and characterized using multinuclear (^{13}C , ^{15}N , ^{19}F) NMR spectroscopy, vibrational (IR and Raman) spectroscopy, mass spectrometry and elemental analysis. The structures in the crystalline state were determined using low-temperature single-crystal X-ray diffraction. The thermal behavior was investigated using differential scanning calorimetry. Quantum chemical calculations for the title compounds and their derivatives containing difluoronitromethyl, fluorodinitromethyl, and trinitromethyl groups have been performed. The gas phase absolute molar enthalpies at 298.15K and 1 atm were calculated theoretically using the modified complete basis set method (CBS-4M) with the Gaussian 09 software. Gas phase standard molar enthalpies of formation ($\Delta H_f^\circ(g)$) at 298.15K were computed using the atomization energy method. Standard molar enthalpies of formation ($\Delta H_f^\circ(s)$) were calculated using $\Delta H_f^\circ(g)$ and the standard molar enthalpies of sublimation (applying Trouton's rule). By using the $\Delta H_f^\circ(s)$ and the densities (for the title compounds determined using X-ray diffraction at 173K and recalculated to ambient temperature; for other compounds estimated) the detonation parameters for presented compounds were calculated using the EXPLO5 V6.02 software. The sensitivities towards impact, friction, and electrostatic discharge were also explored.

Investigations on the energetic performance and thermal stability of N-bonded nitramines

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Keywords: triazole; nitramines; amine; crystal structure; nitrogen-rich.

5,5'-Diamino-4,4'-dinitro-3,3'-bi-1,2,4-triazole is synthesized in a simple and straightforward way by selective nitration of 4,4',5,5'-tetraamino-3,3'-bi-1,2,4-triazole. Moreover, selected nitrogen-rich salts were synthesized and characterized using low temperature single crystal X-ray diffraction. All compounds were investigated by NMR and vibrational (IR, Raman) spectroscopy, mass spectrometry, elemental analysis and DTA. The sensitivities toward impact, friction and electrical discharge were investigated using BAM standards and a small scale electrostatic discharge tester. The detonation parameters were calculated using the EXPLO5 V6.02 code. Heats of formation were computed by the atomization method based on CBS-4M electronic enthalpies. The density, performance, thermal stability and sensitivity of the synthesized compounds were compared to each other and the influence of neighboring nitramino- and amino-groups was investigated.

Investigation of initiating strength of detonators containing TKX-50, MAD-X1, PETNC, DAAF, RDX, HMX or PETN as a base charge

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Keywords: TKX-50; MAD-X1; PETNC; DAAF; underwater explosion test.

An experimental investigation of the initiating capability of detonators containing as a base charge the following explosives: dihydroxylammonium 5,5'-bis(tetrazolate-1N-oxide) – TKX-50, dihydroxylammonium 5,5'-bis(3-nitro-1,2,4-triazolate-1N-oxide) – MAD-X1, pentaerythritol tetranitrocarbamate – PETNC and 3,3'-diamino-4,4'-azoxyfurazan – DAAF in comparison with RDX, HMX and PETN was undertaken. In order to estimate the initiating capability of detonators, the underwater explosion test was applied. The total energy as a sum of the primary shock wave and the bubble gas energies was determined by measuring the overpressure of the shock waves generated in water. Furthermore, the complete synthesis for novel explosives is presented. The thermal behavior of the explosives was explored using differential scanning calorimetry. The gas phase absolute molar enthalpies at 298K and 1 atm were calculated theoretically using the modified complete basis set method (CBS-4M) with the Gaussian 09 software. Gas phase standard molar enthalpies of formation ($\Delta H_f^\circ(g)$) at 298K were calculated using the atomization energy method. In order to obtain the standard molar enthalpy of formation ($\Delta H_f^\circ(s)$) for the prepared covalent compounds, the values of the standard molar enthalpies of sublimation (applying Trouton's rule) were subtracted from $\Delta H_f^\circ(g)$. In the case of salts, $\Delta H_f^\circ(g)$ of ions and the calculated standard molar lattice enthalpies were used to calculate $\Delta H_f^\circ(s)$. The performance parameters (such as heat of detonation, detonation pressure, detonation velocity) based on calculated $\Delta H_f^\circ(s)$ values were computed using the CHEETAH 2.0 software. For the calculations the theoretical maximum densities and densities obtained during the experiments presented in this work were used.

Experimental study on the heat resistant explosive 5,5'-Bis(2,4,6-trinitrophenyl)-2,2'-bi(1,3,4-oxadiazole) (TKX-55): the jet penetration capability and underwater explosion performances

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Keywords: thermally stable explosive; TKX-55; shaped charge; underwater detonation.

The continuous research for new explosives which can resist the high temperatures is driven by strict requirements which must be fulfilled in deep oil and gas drilling applications. In order to fulfill these demands, great efforts have been focused on the development of new thermally stable explosives which are able to resist higher temperatures than hexanitrostilbene and are characterized by superior performance. In the group of recently synthesized thermally stable explosives, 5,5'-bis(2,4,6-trinitro-phenyl)-2,2'-bi(1,3,4-oxadiazole) (TKX-55) is one of the most perspective candidate to be used for a practical application, based on their physico-chemical properties as well as convenient synthesis. Therefore further investigation of the performance of TKX-55 in shaped charge applications was performed. This study is focused on the investigation of the jet penetration capability of the conical shaped charges filled with TKX-55 in comparison to recently used ones. The kinetic energy of the jet depends on the brisance of explosive which is applied. In order to experimentally investigate the shattering effect of TKX-55 the Underwater Explosion Test was applied. Based on the collected data, maximum of overpressure (P_{max}) and time at which the sensor output has decreased to $P_{max}e^{-1}$, the primary shock wave energy (the brisance) was calculated. The determined time interval between the shock-wave pressure peak and the first collapse of the gas bubble was used to calculate the bubble gas energy (the heaving effect). The total energy as sum of primary shock wave and the bubble gas energies was calculated.

Metal nano particle layer deposition by wire explosions

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Keywords: metal nanoparticle; layer deposition; wire electric explosions.

Wire electric explosions (WEE) are of wide scientific interest in the largely investigated field of low temperature plasmas and are found in different applications, such as plasma ignition or the production of nanoparticles. In the latter, electric pulse shape, voltage and current, as well as the wire geometry, fundamentally influence the nanoparticle production and the particle size distribution. Additionally, the surrounding atmosphere allows for the production of different metal compounds like oxides or nitrides. Nanoparticles made of metals and metal oxides can be mixed, forming nano thermite mixtures with high energy release and fast conversion rates. Especially their conversion rate easily exceeds that of micron sized particle thermite mixtures. However, high sensitivity against friction, impact and electrical discharge and agglomeration in the mixing process makes them difficult to handle and process. For experimental investigations, nano thermites have to be deposited on a substrate by mixing with a binder or they have to be filled in glass tubes. In this work, we present an experimental setup for direct deposition of nanoparticles on a substrate by wire explosions. Different wire materials, geometries, and discharge parameters are discussed and analyzed for their mixing ratio and created particle sizes.

Formation enthalpy of trinitrophenol(3-)ion

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Keywords: thermochemistry; enthalpy of formation; calorimetric solution; salt; trinitrophenol.

Thermochemical properties trinitrophenol and its salts of alkaline metals - potassium and caesium are investigated. Complex use of methods of a calorimetry of combustion and dissolution gives the chance not only to define the basic thermochemical parameters of salt compounds - combustion and formation enthalpies, but also to find enthalpies of formation of ions in infinitely diluted water solutions. Besides, these researches allow to raise reliability of calorimetric values at the expense of reception agree values.

Evaluation of the protective systems absorbing the shock wave in the air - testing model

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Keywords: RDX; shock wave; protection.

The paper presents a methodology of research related to the evaluation of the effectiveness and optimization of protection from the damaging effects of explosion and glaring effects of ammunition. The effectiveness of the protection depends on many factors inter alia the material from which the structure was made sheath, the thickness of the individual layers and their relative position to each other. This research will contribute to improving the safety of the uniformed services and professionals at work using explosives and to protect the broader critical infrastructure.

The influence of structure on the thermal decomposition rate of substituted 5,5-dinitro-1,3-dioxanes

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Keywords: 2-R-5,5-dinitro-1,3-dioxanes; kinetics; activation parameters; mechanism.

Thermal decomposition of 2-substituted 5,5-dinitro-1,3-dioxanes is studied in isothermal and non-isothermal conditions. The chemical structure influence on the rate and activation energy is revealed. Decomposition reaction follows the homolytic mechanism and is limiting by the break of C-N or N-N bond depending on the nature of the substituent. Thermal decomposition in non-isothermal conditions flows much faster and is characterized by more large quantities of pre-exponential factor, while the activation energy varies within its definition of error and corresponds to values in isothermal conditions.

Measurement of impact velocity of cladding metal by photonic Doppler velocimetry (PDV)

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Keywords: explosive welding; explosive cladding; PDV; Photonic Doppler Velocimetry.

Explosive welding is a process of reliably joining two different metals often difficult to join by other techniques. The results of the process depend on number of parameters out of which the most important one is the velocity of the cladding metal at the time of impact on the cladded one. This contribution focusses on development of methodology for determination of impact velocity during the welding process. The use of Photonic Doppler Velocimetry (PDV) was tested for this purpose with different types of probes under different angles. Well tested combination in which copper plate was accelerated and welded to the steel baseplate was chosen for conducted experiments.

Determination of the maximum explosion pressure during exposition of organic polymer

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Keywords: explosion characteristics; maximum explosion pressure.

The article deals with the measurement of maximum explosion pressure of organic polymer CR-39 dust cloud. The measurements were carried out according to STN EN 14034-1+A1:2011 Determination of explosion characteristics of dust clouds. Part 1: Determination of the maximum explosion pressure p_{max} of dust clouds. A modified KV 150-M2 chamber was used to measure the monitored characteristics. The organic polymer dust cloud in the chamber is achieved mechanically by high pressure air. The sample is initiated by a chamber nitrocellulose initiator after the spreading of this sample. Immediate initiation of nitrocellulose is achieved by the voltage value which is supplied to the resistance wire. Ignition energy of nitrocellulose used in initiator is 5 kJ. The testing of explosions of organic polymer CR-39 dust clouds showed that the maximum value of the pressure was reached at concentrations of 400 g/m³ and its value is 9.8 bar.

Semicrystalline and domain structure of AMMO/BAMO energetic copolymers

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Keywords: 3, 3-bis(azidomethyl)oxetane and 3-azidomethyl-3-methyloxetane copolymers; block copolymers; X-ray analysis; IR spectroscopy; semicrystalline structure; domain structure.

In the study is investigated the of 3,3-bis(azidomethyl)oxetane (BAMO) and 3-azidomethyl-3-methyloxetane (AMMO) copolymers with a different molecular weight of monomer units, where A is the non-crystallizable "soft" block of AMMO and B is the "hard" block of BAMO, are reported. By wide angle X-ray diffractometry and IR spectroscopy, the amorphous-crystalline structure of AMMO BAMO copolymers is studied; the degree of crystallinity, crystallite size, and their defects are determined. The domain structure of the statistical copolymers is determined using small angle X-ray diffractometry.

Organic molecular explosives impact sensitivity as function of thermochemical parameters and element content

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Keywords: sensitivity; organic molecular explosives; explosion temperature; element content.

The search of new energetic compounds requires preliminary answer about their impact sensitivity earlier than the compound under consideration would be synthesized. Pepekin et al.[V. I. Pepekin et al. Initiation of Solid Explosives by Mechanical Impact. Combustion, Explosion, and Shock Waves, Vol. 44, No. 5, pp. 586–590, 2008] described a simple method to estimate the sensitivity level of molecular organic compounds basing only on its element content and enthalpy of formation. The idea of these method is the assumption that the sensitivity level is linearly correlated with so called maximal heat of explosion. In our investigation it was shown that the correlation with the calculated temperature of explosion at 300 kbar better corresponded with the impact sensitivity level: $P_{cr} = 18.0 - 0.00287 \bullet T_{expl}$, where P_{cr} is the experimental value of the critical pressure of explosion initiation, T_{expl} is temperature of explosion at 300 kbar. Average deviation is ± 0.9

Energy abilities of dinitroderivatives of 1-(trinitromethyl)-1H-pyrazoles as possible oxidizers for solid composite propellants

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Keywords: pyrazoles derivatives; enthalpy of formation; specific impulse; propellant.

As 3,4- and 3,5-dinitro-1-(trinitromethyl)-1H-pyrazoles (C₄H₄N₇O₁₀) have sufficiently high density, (density of 1.906 and 1.937 g/cm³, respectively) with the oxygen balance ($\alpha = 1.18$) they could become quite effective oxidizers for solid composite propellants (SCP) if they have relatively high values of the standard enthalpy of formation ($\Delta H^{\circ}f$). The presence of "non-standard" chemical bonds in molecules under investigation does not allow to rely on estimated values of the $\Delta H^{\circ}f$ values calculated by the additive schemes, and they should be obtained experimentally. The following $\Delta H^{\circ}f$ data were obtained: 3,4-dinitro-1-(trinitromethyl)-1H-pyrazol $\Delta H^{\circ}f = + 261,5 \pm 5.0$ kJ / mol; 3,5-dinitro-1-(trinitromethyl)-1H-pyrazol $\Delta H^{\circ}f = + 246,4 \pm 6,7$ kJ/mol while burning samples in a calorimeter bomb under oxygen in the automatic calorimeter AKS-3M. It has been shown that the use of the compounds under consideration as oxidizer for CSP (as individual compound or with a small amount of AP) allows to achieve values of a specific impulse of 255-260 s with a small amount of aluminum (9-12%) and the hydrocarbon or active binder content of 19% by volume

Preparation and characterization of 3,5-diamino-1,2,4-triazolium 4,4',5,5'-tetranitro-2,2'-biimidazolate (DATNBI)

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Keywords: TNBI; energetic salts; explosive properties.

Ionic derivatives of 4,4',5,5'-tetranitro-2,2'-biimidazole (TNBI) are of growing interest to many researchers these days. Amongst the others, there is 3,5-diamino-1,2,4-triazolium 4,4',5,5'-tetranitro-2,2'-biimidazolate (DATNBI) The salt can be easily prepared from widely available substrates. After filtration and drying, it shows no signs of hygroscopicity and decomposes at 239 °C. The structure of obtained compound was confirmed with NMR spectroscopy and elemental analysis. Thermal properties were investigated with DTA/TG analysis. We also determined standard enthalpy of formation. Detonation parameters were calculated with CHEETAH code for density determined for pressed sample. Some of the energetic properties were measured experimentally.

Crystal morphology and sensitivity of DNTF and FOX-7: Molecular dynamics simulation and experimental study

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Keywords: crystal morphology; DNTF; FOX-7; molecular dynamics simulation; sensitivity.

The growth morphologies of DNTF and FOX-7 in vacuum and different solvent conditions are studied by molecular dynamics simulations based on attachment energy (AE) model. The results indicate that the predicted morphologies of DNTF in H₂O/AcOH and H₂O/EtOH solvent are respectively plate-shaped and rod-shaped, while the predicted morphologies of FOX-7 in H₂O/DMF and cyclohexanone solvent are respectively sphere-shaped and needle-shaped. These are in reasonable agreement with that of observed experimental results. Additionally, the impact and friction sensitivities of DNTF and FOX-7 in different crystal morphologies are also tested and discussed, which implies that the sensitivities of explosives are greatly influenced by their crystal morphology.

Synthesis and characterization of 1,1'-azobis(3,5-dinitropyrazole): a stable, catenated N₆, polynitro energetic compound

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Keywords: energetic compound; 1,1'-azobis(3,5-dinitropyrazole); synthesis; property.

A novel nitrogen-rich, polynitro energetic compound with an N,N-azo linkage, 1,1'-azobis(3,5-dinitropyrazole), has been synthesized and well characterized. The crystal structure was determined by X-ray diffraction. The detonating performance was obtained with density and enthalpy of formation matched with theoretically computed values based on the B3LYP method. The DSC result shows that 1,1'-azobis(3,5-dinitropyrazole) decomposes at a relatively high temperature (239.6°C), which indicates that 1,1'-azobis(3,5-dinitropyrazole) has excellent thermal stability.

Preparation and thermolysis of 1,4-diamino-3,6-dinitropyrazolo[4,3-c]pyrazole

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Keywords: energetic compound; 1,4-diamino-3,6-dinitropyrazolo[4,3-c]pyrazole; N-amination reaction; thermolysis.

1,4-diamino-3,6-dinitropyrazolo[4,3-c]pyrazole (LLM-119) was synthesized by N-amination reaction, and its structure was characterized by NMR, IR, MS and element analysis. The thermal decomposition kinetics and mechanism were studied by means of various heating rate differential scanning calorimetry (DSC), thermolysis in situ rapid-scan FTIR and TG-MS-FTIR coupling technique. The results show that the apparent activation energy and pre-exponential constant of the exothermic decomposition reaction of LLM-119 obtained by Kissinger method are 166.45 kJ mol⁻¹, 1016.53 s⁻¹. The decomposition of LLM-119 included two stages, which begins with the rupture of C–NO₂ with subsequent loss of NO₂ under electron impact and heating condition, respectively. In the first stage of decomposition, the rupture of one C–NO₂ and one pyrazolo ring in LLM-119 molecule with the release of NO₂, HN₃, N₂ and NO occur under electron impact condition, whereas the homolysis of two C–NO₂ bonds occur with the loss of two molecular NO₂ under heating condition. The above research results on thermal behavior is useful for analyzing the stability and thermal safety of LLM-119.

Comparison of kinetics of hyperbranched poly([1,2,3]-triazole-[1,3,5]-triazine)s formation by AB₂ and A₂B type monomers polyaddition

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Keywords: kinetics; azide-alkyne cycloaddition; AB₂ and A₂B type monomers; hyperbranched poly([1,2,3]-triazole-[1,3,5]-triazine)s; degree of branching; regiospecificity; regioselectivity.

Polyaddition kinetics of two azide-acetylene monomers 2-azido-4,6-bis-prop-2-yn-1-yloxy-[1,3,5]-triazine (ABPOT, AB₂ monomer) and 2,4-diazido-6-prop-2-yn-1-yloxy-[1,3,5]-triazine (DAPOT, A₂B monomer) were compared. The study was conducted in the solid phase at the temperature below melting temperature of monomers (by NMR, polarized optic microscopy and SAXS/WAXS technique), in isothermal and non-isothermal conditions in the melt (by DSC), and in the mode of copper(I)-catalyzed azide-alkyne cycloaddition (CuAAC) reactions in DMSO-solution (by IR-spectroscopy). The observed kinetic features and characteristics of hyperbranched poly([1,2,3]-triazole-[1,3,5]-triazine)s were due to differences in the monomers crystal structure for solid phase polyaddition and in the chemical structure of the monomers for solution and melt processes.

Investigation of sodium azide performance in energetic mixtures

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Keywords: sodium azide; detonation performance.

Sodium azide performance in energetic mixtures is investigated. Sodium azide is considered as the main component of the explosive composition or, complementary mixtures of ammonium nitrate with sodium azide are examined. Sodium azide (NaN_3 , SA) is considered as the component enhancing nitrogen content in the explosive mixture. In view of possible practical applications, energetic outcome of considered mixtures was enhanced by addition of aluminium powder. Powdered (Alp) or flaked (Alf) forms of aluminium were considered. Sodium based compounds are expected to form products in gaseous form. As observed detonation velocities of explosive mixtures containing sodium azide are relatively low, in the range of 2000 – 3000 km/s, thermodynamic analysis of chemical composition and evaluation of detonation and explosion parameters was carried out. The obtained results indicate, that despite of relatively low detonation velocity, explosion energy of mixtures containing up to 60 % of SA may attain of 4 MJ/kg or higher.

Nitration of primary amines to form primary nitramines (review)

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Keywords: N-nitration; primary nitramine; literature review.

The nitration of primary amines to form primary nitramines is a rarely reported synthetic procedure which proceeds through a minimum of two steps. This is in stark contrast to the nitration of alcohols and secondary amines which is readily achievable by a number of methods in a single step. In general the primary amine must initially be activated to nitration as direct exposure to nitrating media tends to result in the formation of an ionic nitrate salt. This activation may be achieved through the use of a multitude of protecting groups that are stable to the nitrating conditions used thereafter. The review presented here is an attempt to bring together the published literature on this often overlooked synthetic procedure in energetic materials chemistry.

Kinetic study of the thermal degradation of porous ammonium perchlorate-based composite solid rocket propellant

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Keywords: composite propellant; rubber blocks; ammonium perchlorate; polyvinyl chloride; polyurethane.

Composite propellants are highly solid-loaded elastomers used in solid rocket motor technology. These energetic materials are manufactured by the incorporation of the oxidizing agent and fuel in an organic matrix. During the past 60 years, the thermal decomposition of ammonium perchlorate has been the subject of various research works. Among these research activities, partial decomposition of ammonium perchlorate at low temperature has been observed. This phenomenon permits to produce porous ammonium perchlorate and to use it as an ingredient in composite propellant grains. The aim of this work is to study the effect of porous ammonium perchlorate on thermal properties of rocket composite propellant. The first part of this study consisted for preparing porous ammonium perchlorate (oxidizer) through normal ammonium perchlorate by using a Pyrex cell and followed by the manufacturing of propellant samples using porous ammonium perchlorate and a polyvinylchloride/ polyurethane binders without any other additives. The second part consists on the characterization of propellant systems by ATG and DSC for thermal kinetics evaluation using different kinetic models. From the obtained results we can see that the solid rocket propellants prepared from porous ammonium perchlorate for the both binder (PVC/PU) present the best thermal properties.

The interaction of 1-ferrocenylbutane-1,2,3-trion and 1,1'-ferrotsendiildibutane-1,2,3-trion with substituted hydrazines.

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Keywords: diethyl ether; dinitrophenylhydrazine; ethanol; ferrocene; ferrocenylbutanetrion.

The interaction of 1-ferrocenylbutane-1,2,3-trion and 1,1'-ferrotsendiildibutane-1,2,3-trion with substituted hydrazines. Characteristics and spectral properties of the hydrazone derivatives of 1-ferrocenylbutane-1,2,3-trion and 1,1'-ferrotsendiildibutane-1,2,3-trion **Keywords:** diethyl ether; dinitrophenylhydrazine; ethanol; ferrocene; ferrocenylbutanetrion.

Energies of reorganization of part molecules in radicals

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Keywords: energy of chemical bond; radical; reaction of molecules decomposition; aromatic substance.

On the base of fundamental definitions of chemical physics, the design procedure of energies of chemical bonds and energies of reorganization of fragments of molecules into radicals after unimolecular radical reaction of molecules decomposition have been offered. Energies of reorganization for different compounds of composition $C_nH_mO_pN_q$, including polyradicals and aromatic substances have been determined.

Study on the effect of isocyanates on the PGN cure reaction

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Keywords: elastomer; polyurethane; polyglycidyl nitrate (PGN); binder; isocyanate.

Composite propellant binders are typically cross-linked polyurethanes providing a matrix that hold together a charge of finely divided particles and helps the friendly processing of the energetic materials. The raw polymers are liquid prepolymers with functionally hydroxyl terminated groups. These terminal hydroxyl groups are used for curing with isocyanates to form a polyurethane linkage. The presence of energetic functional groups in the polymer structure allows the composition to have comparatively less explosive filler, thereby rendering less sensation formulation to external stimuli. It is also possible to obtain enhanced performance and improved the energetic properties of propellant formulations, by using energetic binders instead of the inert ones. PGN is one of the new types of energetic polymer which is developed solely for using in propellants. Regarding to the importance of PGN as a suitable candidate for energetic binder purposes, we attempted to follow the course of curing reaction at our study. The purpose of this work is to improve the polymer technology knowledge by studying mechanical properties and thermal behavior of PGN elastomer in presence of different isocyanates. Four different types of curing agents have been discussed in this work, along with their effects on curing reaction and mechanical properties (maximum stress and strain). PGN was cured with fourisocyanate curatives generally employed in composite propellants, viz., Desmudar N-100, TDI, IPDI and HDI, is studied using DSC. Reactions are carried out in presence of DBTDL as catalyst. The tensile properties of the polyurethane elastomers are determined in the different systems is also measured simultaneously and compared with the results from the thermoanalytical DSC method.

Study of aging of double base rocket propellants by microcalorimetry. Assessment of lifespan

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Keywords: double-base rocket propellants; aging; microcalorimetry; lifespan; heat flow.

The present work deals with the assessment of the stability of five double base rocket propellants samples, having various ages. In order to undertake this work, various methods of analysis and characterization of the samples are used, like the high performance liquid chromatography (HPLC) for the qualitative identification and the quantitative evaluation of stabilizers contained in rocket propellants, the FTIR spectroscopy which allows via the detection of the characteristic vibrations of the chemical bonds, to carry out characterization of chemical functions. The essential part of this study consists of an attempt to the development of a methodology allowing the assessment of the stability of double base rocket propellants by using microcalorimetry technique in isothermal mode. A Thermal Activity Monitor (TAM III) device is used for the achievement of experimental work. An important part of the work consists to the evaluation of the lifespan of rocket propellants by using various empirical models available in literature.

Consumption of atmospheric oxygen as ageing indicator of HTPB-based solid rocket propellants

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Keywords: aging; solid rocket propellant; oxygen; raman; fluorescence quenching; quenching.

Changes in material parameters of solid rocket propellants (SRP), which have influence on its in-service-time are considered as ageing. One main reason for ageing is the effect of atmospheric oxygen. In general, oxygen causes additional cross-links within the hydroxyl-terminated polybutadiene (HTPB) binder network, which increase Youngs-modulus. During this process, atmospheric oxygen is consumed by chemical reaction, diffusion and dis-solution. The oxygen concentration in the atmosphere around the SRP sample material is followed with Raman spectroscopy and fluorescence quenching of an oxygen sensitive fluorescence sensor, whereby the latter showed better results. Measurements were performed in a closed vessel and in a sealed model rocket motor in a temperature range from 30 to 90 °C. Appropriate models were applied to describe the reaction kinetics, which underlies the observed decrease of atmospheric oxygen concentration.

Burn rate moderation in composite solid propellants using copper chromite: Influence of oxidation state of copper

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Keywords: copper chromite; composite propellant; burn rate; XRD; XPS; ammonium perchlorate.

Copper chromite (CC) is a well-known burn rate modifier used in composite solid propellants and this acts as a heterogeneous catalyst facilitating the thermal decomposition of ammonium perchlorate (AP) oxidizer. To evaluate the catalytic activity due to synthesis method of copper chromite, two batches of copper chromite were synthesized by pyrolysis at two different temperatures and used in the propellant formulation to study its effect on propellant ballistics. To understand the chemical composition of these batches of copper chromite, detailed characterization was undertaken using chemical methods, particle size distribution by laser scattering, surface area by Brunauer–Emmett–Teller (BET) method, X-ray diffraction (XRD) and as well as X-Ray photoelectron spectroscopy (XPS). Propellant mixing trials were carried in a hydroxyl terminated polybutadiene (HTPB)-ammonium perchlorate formulation by using the copper chromite from these batches and the ballistic properties were evaluated

Phonon spectrum as materials gene for explosive crystals: molecular simulation and thermal property prediction

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Keywords: explosive crystal; phonon spectrum; density functional theory; thermal property.

Phonon is the most important elementary excitation in solid systems, which acts as a kind of materials gene that can determine the heat vibrations and thermal properties in the molecular crystals. The phonon spectrums of typical explosive crystals β -octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) without π -stacking and 1,1-diamino-2,2-dinitroethene (FOX-7) with wave-like π -stacking were obtained by molecular simulation and calculations. As results, it was found that the peaks at low frequency are comparable with experimental and the molecular vibrational modes are in agreement with previous reports. Thermodynamic properties including Gibbs free energy, enthalpy and heat capacity as functions of temperature were obtained based on the calculated phonon spectrum. The heat capacity at normal temperature was calculated using linear fitting method, with a result consistent with experiments. The results are of importance to investigate the physical nature of crystal stability and molecular bond dissociation mechanism in the explosive detonation, which is strongly related to molecular and lattice vibrations.

Coordination derivatives of 4,4',5,5'-tetranitro-2,2'-biimidazole (TNBI) as new complex explosives

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Keywords: complex explosive materials ; tetranitrobiimidazole ; coordination explosive materials.

The aim of this project was to obtain new explosive materials which could be used for military purposes. We successfully synthesized with high yield and purity coordination explosives containing metals such as copper (CuTNO), nickel (NiTNO), cadmium (CdTNO), cobalt (CoTNO) and zinc (ZnTNO) as the central atoms, ammonia and water molecules as ligands and anion which was 4,4', 5,5'-tetranitro-2,2'-biimidazole (TNBI). Materials were tested with spectroscopic methods such as nuclear magnetic resonance, infrared spectroscopy and Raman spectroscopy. Thermal properties were examined by differential thermal analysis, thermogravimetry and differential scanning calorimetry. The purity of the compounds was deduced from its elemental analyses.

New explosive coordination compounds based on 2,2'-azotetrazole

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Keywords: coordination compound ; azotetrazole ; coordination explosive materials.

In this work we successfully synthesized complex explosive materials containing metals such as copper (CuAZT), nickel (NiAZT) and cadmium (CdAZT) as the central atoms, ammonia and water molecules as ligands and 2,2'-azotetrazole as an anion. The compounds were obtained with high yield and purity in aqueous environment. Products were characterized by spectroscopic methods such as multinuclear magnetic resonance (¹H, ¹³C NMR), infrared spectroscopy (FTIR) and Raman spectroscopy (RS). The sensitivity for friction and impact were determined according to BAM standards. Thermal properties were determined with differential thermal analysis (DTA), thermogravimetry (TG) and differential scanning calorimetry (DSC). The purity of the compounds was confirmed with elemental analysis.

Synthesis and properties of a silicon containing nitrocarbamate based on pentaerythritol

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Keywords: energetic materials; nitrocarbamates; silanes; neopentane; crystal structure.

The new silicon containing nitrocarbamate tetrakis(nitrocarbamoymethyl)silane (sila-PETNC) has been synthesized in several steps starting from silicon tetrachloride. The compound and its carbamate precursor have been comprehensively characterized, including ^{29}Si NMR spectroscopy. Both the carbamate and the nitrocarbamate structures could be confirmed by X-ray diffraction. In addition, detonation performances were calculated by computed enthalpies of formation and the EXPLO5 code. Finally, the energetic properties of sila-PETNC were compared with its carbon analogue PETNC and their nitrate esters sila-PETN and PETN, respectively.

The effect of an annular boric acid layer on the shock wave generated by explosive charge detonation

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Keywords: boric acid; blast mitigation; pressure.

The experimental tests presented in this paper consisted in a series of detonations of small cylindrical explosive charges in the presence of an exterior layer of boric acid for various explosive/acid mass ratios. Pressure transducers were used to measure overpressure and a high speed camera was used to record images during the phenomenon. The tests results indicated mitigation of both maximum overpressure and impulse. The experimental data expressed as functions of the relative distance, Z , are consistent, showing a decreasing tendency of the attenuation. The high speed camera data indicated a rapid quench of gaseous products and the inhibition of burning processes.

Phosphorus oxonitrides as one of the key components of the intumescent systems

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Keywords: phosphorous oxonitrides; intumescent systems.

The composition of coke formed by heating the intumescent mixture based on ammonium polyphosphate and pentaerythritol was studied. A comparative analysis of the outer surface and an inner layer of coke is presented. It was found that the outer surface of coke initially is quite hard armor, but over time, becomes loose. Most likely products formed by the combustion of air humidity hydrolysed. According to photoelectron spectroscopy in addition to the main line $2p_{3/2}$ (134.80 eV) in the spectrum of the outer layer contains two lines with anomalously high binding energies - 137.07 eV (9%) and 139.87 eV (4%). According to IR spectroscopy, together with the absorption band at 923 cm^{-1} ($\nu\text{P-O-P}$) and 1252 cm^{-1} ($\nu\text{P}=\text{O}$) intense absorption band at 1000 cm^{-1} , attributed to the vibrations of $\nu\text{P}\equiv\text{N}$, is present. It is assumed that the resulting oligooksonitrides besides providing the mechanical strength and heat resistance of the coating prevent the penetration of air oxygen into coke, thus ensuring the formation of CO and its subsequent disproportionation to carbon and carbon dioxide according to Boudoir reaction.

Selected properties of heterogeneous solid rocket propellant based on HTPB after accelerated ageing

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Keywords: heterogeneous solid propellant; accelerated ageing.

A study has been performed with an HTPB propellant to determine changes in its properties after ageing. During spontaneous ageing this materials are subjected to various degradation reactions. In this case research has been carried out by accelerated ageing technique in elevated temperature. By using this method propellant behavior during ageing was simulated over a shorter period of time. The investigation was made on most important properties: hardness of the propellant, plasticizer and soluble fraction content, crosslinking density, impact and friction sensitivity, decomposition temperature and heat of combustion. The blocks of propellant were hermetically sealed in aluminium foil. The analyses are made for both unaged and aged samples. Methods of measurements were described and analysis of results. Research was made in order to show the relationship between properties of heterogeneous solid rocket propellant and time of ageing and to define which of them are mostly affected by ageing

Initiation of explosive transitions in energy-saturated cobalt salt and nanosized carbonic additives compounds by means of high current electron beam

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Technology (Technical University)

Keywords: cobalt energy-saturated complex; high-current electronic beam.

Experimental research of the high-current electron beam initiation of explosive transitions in energy-saturated complex taken on the base of cobalt amminat and nanosized carbonic additives such as fullerene S60 and detonation synthesis nanodiamonds is performed in the work.

Numerical simulation of explosively driven aluminum flyer acceleration

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Keywords: numerical simulation; LS-DYNA; acceleration; flyer; Explo5.

The acceleration of explosively driven aluminum flyer was successfully simulated using LS-DYNA code. The properties of the explosive (A-IX-1, RDX/binder 95/5) was completely calculated by Explo5 program (detonation velocity and pressure, JWL parameters for the expansion isentrope). The results were compared to the experimentally obtained velocity profile, measured previously with PDV. The both curves agree by shape, velocity values at the individual steps and their duration. Also the terminal velocities agree very well.

Effect of Butacene on ageing of composite propellants

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Keywords: Butacene®; composite propellant; DMA loss factor; TMA glass-rubber transition; van't Hoff rule.

High burning rates together with a low pressure exponents (n) are the effects of Butacene® when used in conventional HTPB based propellant, which is known since the 1980's. A detailed accelerated aging program based on thermal equivalent load established with the generalized van't Hoff (GvH) rule was started to investigate the effect of BUTACENE®, which is a product of SNPE, France. BUTACENE® has ferrocene grafted to regular HTPB backbone. For the final propellant, a special type of vulnerability is reduced, since migration of ferrocene type burning catalyst is suppressed via this grafting. Ferrocene (ferrocenyl-4 butyl dimethyl silane) attached to or in close proximity to HTPB makes it prone to crosslinking with the available atmospheric oxygen, because iron is an oxidation catalyst. This effect may lead the different failure mechanism in the propellant grain constrained under different loads, such as in rocket motor cases. Thermal, mechanical and morphological techniques were used to evaluate the effect of BUTACENE® during an accelerated aging program of AP/Al/HTPB-IPDI based propellants. Comparison of TMA linear thermal expansion curves versus measurement temperature revealed similarities to DMA loss factor curves. The latter show distinguished peaks in going from low to high temperatures due to molecular re-arrangements on the molecular level taking place in different binder fractions. DSC failed to show such re-arrangements in the polymeric network, it only reveals the free or unrestricted polymer chains' glass-rubber transition temperatures (T_g). Infrared spectroscopy was used to follow aging of the formulations where certain bonds disappeared at the end of strong accelerated aging (i.e., at 80°C for 48 days). GvH and Arrhenius type parameterizations were used to evaluate the chemical in-service life of the BUTACENE® based composite propellants and a comparison is provided.

Preparation of spherical energetic composites and their thermal decomposition kinetics

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Keywords: FOX-7; AP; composites; thermal decomposition.

Burning rate depressant is of significant importance for the development on a long-range rocket. Recent works have attracted a lot of attention for a new possibility of 1,1-diamino-2,2-dinitroethene (FOX-7) to depress a burning rate. Furthermore, the introduction of FOX-7 huge-ly decreases the propellant burning temperature. In this respect, FOX-7 is a promising high en-ergetic material that is very useful for the modification of the burning rates of ammonium per-chlorate (AP)-based propellants. In this work, the spherical FOX-7/AP composites are prepared by the crystallization combined with agglomeration that is greatly influenced by the amount of bridging liquid and the agitation rate; thus, their effects on the average size of the FOX-7/AP composites are experimentally investigated. It was found that size of the FOX-7/AP compo-sites increased with amount of the bridging liquid which was used as an agent for agglomera-tion. Size of the composite particles was also increased when the agitation rate was increased from 300 to 400 rpm, but, tended to decrease over 400rpm. The TG curves clearly showed that the presence of FOX-7 enables the 70–90 wt% of AP to decompose at the LTD state, and the activation energy was found to decrease remarkably at the HTD state.

Production of bengal stick sparklers from old single and double base propellants

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Keywords: long term stored propellant; pyroxylin; bengal sticks; sparklers; additives.

It was investigated the application of waste, long-term stored single - base propellants (SBP) and double base propellants (DBP) for obtaining of Bengal sparkler sticks. The activation energy of evaporation of the solutions of SBP and DBP and additives were determined. The elemental analyses of propellants were made. The technology for the production of Bengal sparkler stick was made. It was simple and was easy for application. The prices of the Bengal sticks were determined. In this way some part of waste, long-term stored single base and double base propellants were utilized.

Study on thermal behaviour of AP/LiBH₄ energetic system by heat flow calorimetric method

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Keywords: energetic system; heat flow calorimetric; compatibility; thermal decomposition; property.

High energy density compound ammonium perchlorate (AP) and strong exothermic LiBH₄ represent respectively an excellent principal explosive and a kind of perfect fuel. Thermal compatibility plays an important role and is first considered in the design of novel energetic system. Heat flow calorimetric(HFC) was used to study thermal decomposition of AP, LiBH₄ and AP/LiBH₄ energetic system on a micro calorimeter C80 to provide a beneficial guidance. The thermal characteristics of AP/LiBH₄ is obtained and compared with the single component. The experiment shows that AP does not decompose at low temperature less than 100°C. AP/LiBH₄ energetic powder system decomposes at 59.7°C and advances 4.6°C than pure LiBH₄. Exothermic reaction is demonstrated for both LiBH₄ and AP/LiBH₄. The decomposition of AP/LiBH₄ at low temperature is mainly expressed as the decomposition of LiBH₄. No obvious heat chemical reaction between AP and LiBH₄ during heating process under 100°C demonstrates the compatibility of AP and LiBH₄. All these support HFC method suitable to study the compatibility between AP and novel energetic material LiBH₄. This research may offer effective reference in design of novel energetic formula and provide potential novel energetic system in mixed explosives.

Evaluation of nitromethane as an ingredient in gelled propellants

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Keywords: nitromethane; monopropellant; impact sensitivity; gelled propellants; CNTs.

Nitromethane, the simplest nitroalkane, is studied as a monopropellant since nearly 70 years. In this paper enthalpies of formation are calculated and compared with available measured data and based on this the resulting specific impulses are calculated. Also, the impact sensitivity of nitromethane is studied and the influence of the sample preparation on the results is shown. Nitromethane has a melting point frequently too high for use as a monopropellant. To overcome this drawback, additives for decreasing the melting temperature have been evaluated. . Additives are nitroalkanes, classic solvents and a dinitramide based energetic ionic liquid (EILs). Commercial CNTs as gel agents for nitromethane are evaluated and different deagglomeration methods are tested.

Thermobaric effect comparison of cast thermobaric PBX and TNT in enclosure test

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Keywords: thermobaric explosive; PBX; TNT; enclosure test; shockwave overpressure.

This paper reports on the examination of thermobaric effect of explosives by measuring the shockwave parameters at different distances in a reinforced enclosure. Parameters of the shock wave in air are measured and compared for cast TNT and cast cured thermobaric PBX explosives. Thermobaric explosives containing HMX, ammonium perchlorate, aluminium, magnesium, boron and HTPB binder are prepared by casting technology, and experimental samples are prepared of 400g weight and 50 mm in diameter, without casing. Density and velocity of detonation for the examined cast explosives are determined. Shockwave overpressure was measured using piezoelectric probes placed at the same height as the explosive samples, at different distances from the center of detonation.

Influence of polyacrylamide and stearic acid on crystal growth of RDX

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Keywords: RDX; crystallization; polyacrylamide; stearic acid.

Cooling and antisolvent crystallizations of RDX from acetone solutions were performed. In the case of addition of stearic acid during cooling crystallization more spherical and bit less impact sensitive crystals were obtained. If 0.1% of polyacrylamide-water solution is continuously added to acetone–RDX solution, less friction sensitive and relatively smooth crystals should be obtained. Other tested additives (polyacrylic acid, polyvinylpyrrolidone, guar gum and waxes) had not significant positive effect. RDX samples of relatively spherical crystals are promising candidates for less sensitive PBX or as a starting material for reduced sensitivity RDX.

Impact sensitivity investigations of individual explosives: comparison of the different experimental evaluations

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Keywords: impact sensitivity; structure of compounds ; estimation; comparison of methods.

Statistical processing of experimental data on the impact sensitivity of explosives is carried out. Comparison of estimations accuracy of the methods recommended by the United Nations for the risk level evaluation of dangerous loads during transportation is conducted. It is shown, that despite of some differences in methodical approaches, all methods presented in «Recommendations of the United Nations» give the similar results. It is noted, that for HEM-s with the temperature of melting $<100^{\circ}\text{C}$ (so-called meltable ones) the drop weight test give obviously underestimated risk levels. At the same time for compounds with the temperature of melting $> 250^{\circ}\text{C}$ (so-called heat-resistant ones) the risk levels obtained in the tests on drop weight machines are obviously overestimated. It is connected with the specificity of the tests on drop weight machines.

A novel triazolotriazine-carbonitrile and related molecules

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E. Chavez, Jacqueline M. Veauthier, R. Jason Scharff**

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Keywords: triazole; triazine; carbonitrile; 3-amino-5-cyano-1,2,4-triazole; nitroacetonitrile.

Diazotization of 3-amino-5-cyano-1,2,4-triazole followed by treatment with nitroacetonitrile leads to the formation of the novel fused-ring heterocycle triazolotriazine-carbonitrile. Functionalization of the $C\equiv N$ bond in TTC leads to the formation of two new triazolotriazines that are substituted with either a tetrazolyl or a N-hydroxyamidinyl substituent. The new fused-ring heterocycles are presented along with the spectroscopic, crystallographic, and energetic properties of the materials.

New energetic compound – bis(4''-nitro-[3,3':4',3'']-trifurazan-4-yl)-diazene

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Keywords: furazan; nitrofurazan; azofurazan; 1,2,5-oxadiazole; 3,4-bis(4-nitrofurazan-3-yl)furazan.

Using 3,4-bis(4-aminofurazan-4-yl)furazan (BATF) as a starting material novel energetic compound – bis(4''-nitro[3,3':4',3'']trifurazan-4-yl)-diazene (BNTFDA) was synthesized. The titled compound was prepared by three stages synthesis from 3,4-bis(4-aminofurazan-4-yl)furazan (BATF). The synthesis includes oxidation of BATF by 35% hydrogen peroxide in concentrated sulphuric acid to 3,4-bis(4-nitrofurazan-3-yl)furazan (BNTF), substitution of one nitro group of BNTF to amino one by the action of ammonia and further oxidation of thus prepared 4''-nitro[3,3':4',3'']trifurazan-4-amine (ANTF) by KMnO₄. The structure of BNTFDA was characterized by IR, NMR, MS spectra, X-ray diffraction analyses and elemental analysis. The compound melting point is 117 oC, maximum decomposition point is 296 oC, crystal density is 1.800 g•cm⁻³, shock and impact sensitivity is similar to HMX.

Numerical modeling of thermal initiation of explosives

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Keywords: explosives; thermal initiation; cook-off; finite difference method; reactive heat conduction; energy balance equation.

During their production, handling, and use, explosives and munitions can be exposed to a variety of unplanned thermal stimuli. Heat energy absorbed from surrounding heat source leads to exo-thermic chemical decomposition of an explosive and can, under certain conditions, result in so-called thermal explosion. Because possibilities of such events are of great concern among explosives' community, many theoretical, experimental, and simulation studies have been done in the past few decades exploring the thermal initiation phenomenon. Attempts are directed towards development of reliable numerical models capable of predicting response of explosives to thermal stimuli. Such predictive tools will enable reduction of costs associated with necessary testing and will give additional insight into the thermal behaviour of energetic materials. In this paper we present in-house one-dimensional reactive heat transfer code aimed to model various thermal insult scenarios associated with explosives. The code predicts the transient temperature distribution, the time to ignition, and the location of ignition. The code uses the finite difference method and has built-in self-adjustable time step, various reaction rate models (single-step and multi-steps), and composition- and temperature-dependent thermophysical properties. The results of calculation are compared with literature reported experimental data on cylindrical nitrocellulose specimen and spherical specimens (One-Dimensional Time to Explosion, ODTX, test) for several explosives. Special attention is given to analysing the effect of reaction kinetics on calculation results.

Synthesis, LC-MS analysis and preliminary investigation of some properties of novel 1,3-dihydro-2H-benzimidazol-2-one nitro and nitramino derivatives

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Keywords: 1,3-dihydro-2H-benzimidazol-2-one; nitrocompounds; nitramines; high energy materials; synthesis; LC-MS analysis; X-ray diffraction; properties.

Synthesis and properties of series of novel 1,3-dihydro-2H-benzimidazol-2-one nitro and nitramino derivatives are described. The nitration reactions and purity of synthesized products were analyzed by LC-MS method. A detailed structure of one of the obtained compounds, 4,5,6-trinitro-1,3-dihydro-2H-benzimidazol-2-one (TriNBO) was characterized using low temperature (173 K) single crystal X-ray diffraction: orthorhombic yellow prism, space group 'P 2 21 21', experimental crystal density 1.767 g/cm³ (at 173K). The TriNBO contains a one activated nitrogroup in the 5-th position, which was used for the nucleophilic substitution in the aminolysis reactions with methylamine, ethylamine, n-propylamine and ethanolamine. The obtained aminoderivatives were nitrated with N₂O₅/ HNO₃ and resulted a group of new appropriate nitramines: 1,3-dihydro-2H-5-R-N(NO₂)-4,7-dinitrobenzimidazol-2-ones. These derivatives were investigated using LC-MS analysis and characterized by spectroscopical (UV, IR, ¹H and ¹³C NMR methods). Thermal analysis (TGA) of three selected representatives was done. The most of novel compounds possess a high melting points (200-315 °C) and thermal stability and can find a potential application as new thermostable energetic materials. Some calculated preliminary energetic characteristics show that TriNBO, 5-methylnitramino-1,3-dihydro-2H-4,7-dinitrobenzimidazol-2-one and 5-nitratoethylnitramino-1,3-dihydro-2H-4,7-dinitrobenzimidazol-2-one possess an increased energetic characteristics in comparisson with TNT. The proposed nitrocompounds may find a potential application as thermostable high energy materials.

Numerical simulation of blast loaded Ti/Steel foam/Ti sandwich plate

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Keywords: ballistic protection; steel foam; sandwich structures.

During blast events the overpressure generated by high explosives detonation acts on every structure that blast wave encounters. As a result, the structures exhibits high strain rates and thermal loadings. In order to estimate if a structure, especially the ones used in ballistic protection, will withstand the blast wave, experimental or/and numerical simulation investigations must be carried out. The present paper aims primarily to investigate, by numerical simulation means, the behaviour of a Ti/Steel foam/Ti sandwich plate loaded by a blast wave. Also, using LsDyna commercial software, a comparative study between a simple steel armour plate and the Ti/Steel foam/Ti sandwich plate is performed. The study results points towards the idea that the sandwich structures could prove itself a good choice for certain application.

Physicochemical properties of erythritol tetranitrate and its solutions in nitroglycerine and diethylene glycol dinitrate

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Keywords: erythritol tetranitrate; nitroglycerine; diethylene glycol dinitrate; solid-liquid diagrams.

Physicochemical properties of erythritol tetranitrate and its solutions in nitroglycerine and diethylene glycol dinitrate have been studied. The purity of erythritol tetranitrate has been studied, the value of enthalpy of melting and thermal stability have been determined, and the solubilities of erythritol tetranitrate in nitroglycerine and diethylene glycol dinitrate have been studied using differential scanning calorimetry. The purity of the tetranitroester is 99.607 ± 0.174 mol %. The enthalpy of melting is 123.9 J/g. An equation has been derived for the constant of ETN thermal decomposition. In an isothermal mode (at 70°C), the decomposed tetranitroester amount does not exceed $4.43 \cdot 10^{-3}$ wt % in 60 minutes. The vaporization of the tetranitroester has been studied by thermogravimetry. Erythritol tetranitrate experiences two processes under heating: decomposition and vaporization. It vaporizes more rapidly than decomposes. Solid-liquid diagrams have been plotted for erythritol tetranitrate-nitroglycerine and erythritol tetranitrate-diethylene glycol dinitrate systems. At room temperature ($t=20^\circ\text{C}$) nitroglycerine and diethylene glycol dinitrate dissolve about 16 mol % erythritol tetranitrate. The properties of erythritol tetranitrate-nitroglycerine and erythritol tetranitrate-diethylene glycol dinitrate two-component solutions have been ascertained. These two-component solutions have higher densities and lower volatilities than individual nitroglycerine or diethylene glycol dinitrate. The two-component solutions are completely thermodynamically compatible with polyurethane and divinyl nitrile rubbers. Keywords: erythritol tetranitrate; nitroglycerine; diethylene glycol dinitrate; solid-liquid diagrams.

A review of the mallet impact test for small scale explosive formulations

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Keywords: impact test; small scale explosive formulations.

Development of new explosive formulations begins with the generation of only a few milligrams of material which is investigated using a number of small scale tests such as DSC, TGA, response to flame, mallet impact (mallet friction either glancing or direct blow) to determine whether the formulation is safe to scale up to 10 g. The latter of these tests, mallet impact, can be particularly subjective as the result is directly influenced by the operator carrying out the assessment. Not only can there be a change from one operator to another but there can also be a change in the force applied during each strike potentially leading to inconsistent results. This study highlights this encountered variation and assesses the load applied by a variety of operators with varying levels of explosive experience. This paper also proposes the use of a small scale laboratory based impact test which would provide improved confidence in the assessment of impact sensitiveness of explosive formulations and assist in justifying whether a formulation can be taken to the next scale. A small scale version of the BAM impact test (EMTAP Test 43) has been devised that allows the comparison of the sensitiveness of small scale formulations relative to RDX (8.7 J, EMTAP Test 43B) whilst also ensuring a reproducible result.

Jet flow simulation of nano CL-20 explosive ink

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Keywords: explosive ink; direct writing; jet velocity.

Nano CL-20 explosive ink based on direct writing technology was applied for micro-charge of the micro-detonation sequence of MEMS micro-initiators. Direct writing of CL-20 explosive ink is the ink flow driven by nozzle pressure and rapid solidification. In order to study the effect of the influences of pressure, needle diameter and ink viscosity on the process of direct writing a simulation model of direct writing jet of CL-20 explosive ink was set up. FLUENT, numerical simulation software was applied to simulate the changes of ink jet velocity under the different pressure, needle diameter and ink viscosity. The simulation results showed that the fluid velocity in nozzle increased proportionally when the pressure rose. Moreover, the ink viscosity increased while the velocity fell and its range decreased. With the increase of nozzle diameter, the ink velocity rose and its range augmented.

Molecular dynamic simulation of CL-20/FOX-7 co-crystal explosive

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Keywords: co-crystal; molecular dynamics; 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane.

Seven models of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) /1,1-diamino-2,2-dinitroethylene(FOX-7) co-crystal were constructed based on the hydrogen bond rules of co-crystal formation. The probability of CL-20/FOX-7 co-crystal formation was investigated using the molecular dynamics (MD) method. The results show that the orders of binding energies of the seven co-crystal models are $E_b(1\ 0\ 1) > E_b(1\ 1\ -1) > E_b(\text{randomness}) > E_b(0\ 1\ 1) > E_b(0\ 0\ 2) > E_b(1\ 1\ 0) > E_b(1\ 0\ -1)$, the intermolecular forces of the model that CL-20 molecular substituted by FOX-7 on the surface (1 0 1) and (1 1 -1) of CL-20 is stronger than other models, and the XRD peaks of seven co-crystal models are quite different from pure CL-20 or FOX-7. It can be predicted that CL-20 molecule would be more easily substituted by FOX-7 on the surface (1 0 1) of CL-20 to obtain the stable co-crystal structure in the preparation of the CL-20/FOX-7 co-crystal explosive.

Synthesis and detonation properties of series of high nitrogen macrocyclic compound

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Keywords: macrocyclic; synthesis; detonation properties.

Abstract Series of aromatic macrocyclic compound with a large number of nitro groups are synthesized. They were obtained by the reaction of [2+2] into the ring. With the increase of the number of nitro group, the detonation velocity and detonation pressure of the large ring compound increased significantly, and the density of the crystal was also significantly larger. Keywords: macrocyclic, synthesized, detonation properties

Tuning reactivity of nanoaluminum with fluoropolymer via electrospray deposition

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Keywords: nanoaluminum; fluoropolymer; electrospray deposition; reactivity; energetic materials.

Fluoropolymers are a class of potent oxidizers for aluminum powders due to the strong electronegative fluorine within these polymers. What is more, some of them are also the excellent binder. Herein, the Polyvinylidene Fluoride (PVDF) is selected as the reactive binder of nanoaluminum (n-Al) to fabricate n-Al/PVDF microsphere particles using the electrospray deposition method. The size of these close-grained spherical particles at 1 μ m to 5 μ m was successfully prepared with binder content of 5%, 10% and 15% by mass. When increasing the PVDF content to 15%, the polymer fibers appears. Thermogravimetric-differential scanning calorimetric (TG-DSC) analysis in oxygen-argon mixture atmosphere shows that the onset and peak temperature of microsphere particles at main exotherm is postponed compared to n-Al. However, these particles show more intense heat release process (the sharper exothermic peak). The combustion properties tested in open air show that all samples can be ignited, while the n-Al/PVDF demonstrated the more intense reactivity (dazzling flame and a lot of sparks, especially for the 15% PVDF sample) in comparison to n-Al. The work, which shows that using electrospray deposition fabricates the spherical particles which are consisted by n-Al and reactive binder, expects an approach to the vast application of n-Al in energetic materials.

Novel formulations of ballistic gels for shock wave impact behavior determination

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Keywords: forensics; materials; ballistics; shock wave.

Forensic ballistic tests involve the use of various ballistic gelatins and soaps. Their use is restrained due to several important factors: their synthesis strategy, their availability at room temperature and their rapid degradation even when kept in cold places. The importance of human torso surrogates translates in the facility to verify various ballistic factors impact, such as shock wave or fragments. In the first case, the use of PVDF sensors inside torso surrogates helps in defining safety distances and materials for individual protection equipment.

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