Abstracts of the 25th Seminar on

New Trends in Research of Energetic Materials

NTREM

Pardubice, April 19–21, 2023

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Institute of Energetic Materials

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Held at the University of Pardubice

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

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Preface

The International Seminar New Trends in Research of Energetic Materials (NTREM) has traditionally been an international meeting of students and early-career researchers involved in the research, development, technology, or industrial application of energetic materials.

It started as a local meeting organized by Research Institute of Industrial Chemistry in Explosia in 1999 with the aim of teaching the youth scientists to present the results of their work to a professional audience. Students from the Institute of Energetic Materials took part in the event and found it useful to their professional development. Therefore, it was decided to continue with these seminars and hand over their organization to the University of Pardubice.

Under the enthusiastic leadership of Prof. Zeman, this local meeting developed over the 25 years to a well established international event. While growing in size, it maintained its original focus and always aimed to give students and newcomers to the field of explosives the ability to present their work even in the early stages of development and to build personal relations with colleagues from countries all over the world.

The 25th NTREM seminar featured a diverse range of topics while maintaining its traditionally strong emphasis on synthesis. The seminar proceedings contain papers presented at the event either in oral or poster form.

I would like to take this opportunity to express my sincere gratitude to the generous sponsors for their support. Their financial assistance was invaluable in making this event possible and allowed us to keep the registration fee at a minimal level. The seminar was supported by the following:

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I also express my deep gratitude to the members of Scientific Committee, the Organizing Committee, the authors of all the seminar papers and, finally all the participants of this seminar.

Pardubice, March 20th, 2023 Jiri Pachman

Comparison of castable PBXs prepared from different sources of energetic fillers in terms of processability

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Keywords: polymer bonded explosive; curing behavior; end-of-viscosity.

Castable polymer-bonded explosives are typically formed by energetic fillers and a polymer matrix consisting of a binder, plasticizer, and curing agent. The processability and castability of polymer-bonded explosives into the warheads become easier when the end-of-viscosity is in the desired range. The end-of-viscosity of a polymer-bonded explosive is affected by several factors such as solid loading (w/w), particle size distribution (fine/coarse ratio), and particle shape (sphericity) of energetic fillers. In this study, polymer-bonded explosives were produced by using energetic fillers supplied by three different sources. Different end-of-viscosity and pot life have been observed with the same formulation of polymer-bonded explosives. In order to understand the reason behind this, explosives were produced and evaluated with altered design parameters. The source of energetic fillers, solid loading, morphology, particle size distribution (fine/coarse ratio), and pre-coating of energetic fillers, are taken into consideration as the design parameters.

Chemistry of 2-hydroxy-5-aminotetrazole

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Keywords: tetrazoles; functionalization; X-ray diffraction; salt formation.

Tetrazoles are a unique class of endothermic and highly energetic compounds that can be used in all classes of energetic materials as a) explosives, b) propellants as well as c) pyrotechnics. 1-hydroxy-5-aminotetrazole is a well-known nitrogen-rich tetrazole compound that has been utilized for numerous derivatizations e.g. nitration, oxidation through azo-coupling or salt formation. It can be synthesized through the reaction of cyanogen azide with hydroxyl amine in poor yields or more recently via O-benzylhydroxylamine, cyanogen azide, and subsequent reductive deprotection in much better yields. Despite the simplicity of its isomer, 2-hydroxy-5-aminotetrazole, the compound is not reported. In this study, 2-hydroxy-5-aminotetrazole and selected derivatives are characterized in terms of their chemical and energetic points of view. Several energetic salts based on 5-aminotetrazol-2-oxide anion are investigated. All compounds were intensively studied through multinuclear NMR and IR spectroscopy, X-ray diffraction experiments, thermal stability testing using DTA, and sensitivity measurements according to BAM standards. The detonation performances were calculated using the EXPLO5 code.

Chemical stability and thermal analysis – use of terms and methods with energetic materials

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Keywords: chemical stability; thermal analysis; instrumentations; reaction models; optimal model.

Energetic materials (EM) tend to decompose in thermodynamically more stable substances. The rate of chemical degradation is not equal for all the types of EM. By experience the so-called nitrate esters as nitrocellulose, nitroglycerin, iso-propylnitrate and others are pronounced less stable, means degrade faster, than RDX, HMX, TATB, FOX 7 and others. The reason is found in the chemical structure, in the values of bond dissociation enthalpies and the possibility to be attacked by relative reactive reactants as water, oxygen, acids, and bases. Because the rates of decomposition are largely different, a separation based on the decomposition rates has developed into mainly two groups using own terms, instrumentations and reaction kinetic descriptions. For the assessment of the faster decomposing substances, the general term 'chemical stability' is used. With slow rate decomposing substances, the term 'thermal analyses' is the appropriate one. Instrumentation and kinetic descriptions will be presented and contextualized. For finding the adequate model to describe the data, the evaluation with regard to lowest number of model parameters is a preferred option, whereby the so-called information criteria can help to find the best model.

Fifty years development in the thermodyamics of ideal condensed phase detonations

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Keywords: ideal detonation; computational modelling; EOS; model.

Over the last fifty years since the development of perturbation theories for condensed phase thermodynamics, reliable computational procedures for the properties of detonation product molecules have been developed. Empirical (e.g. BKW EoS) and semi-empirical (JCZ3 EoS) have been largely replaced by approaches based on sound statistical mechanical theories incorporating a fixed set of fundamental physico-chemical parameters. The parameters chosen for a three-term repulsive potential are in agreement with shock Hugoniot data, corresponding states principles and also include the role of attractive forces in polar molecules (e.g. water, ammonia). Of importance to the CFD/FE community, isentropic data and their derivatives are well-behaved and without the anomalies of earlier simulations.

The original development of software for these more realistic EoS initially required some hours on supercomputers for a single study. With the use of Chebychev polynomial fits and refined SQP methods, these times have been reduced to a few seconds on a conventional laptop computer.

This paper will address the current state of ideal detonation physics and also address some remaining uncertainties in these models.

Optimized parameters for underwater blast wave generator models used in design of protective structures

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Keywords: underwater blast wave generators (WBWG); small scale blast tests; optimized JWL parameters; thermochemical code THOR; Autodyn 2D predictions.

Underwater blast generators (WBWG) are formed by an explosive charge detonated inside a water container. They are used more and more to design protective structures as they have an extremely high rate of conversion of the explosive detonation energy into the kinetic energy of a thick water confinement compared to air blast effects. The protective structures are generally formed by steel frame and steel plates. These and other types of plated blast protection elements can be analyzed in small-scale blast tests using WBWGs. The study starts with the selection of high explosives and the review of their detonation properties and model parameters. Later on, the water shock transmission properties are discussed. Our study is focused on numerical methodology that would support an experimental evaluation of plate performance subjected to WBWG. Selected explosive charges are PBX (Plastic Bonded Explosive), PETN (PentaErythritol TetraNitrate) and Ammonium Nitrate emulsion explosive. The performance of these explosive compositions is defined on the basis of theoretical and experimental studies conducted at University of Coimbra in the past two decades. Prediction of their detonation properties was done using in-house thermochemical computer code THOR. Further, the Jones-Wilkins-Lee equation of state was chosen for definition of expanded detonation products. The material and shock constants were implemented in Autodyn, the created model was compared to THOR calculations and acquired experimental data, and the evolution and the attenuation of the detonation wave in different material domains are evaluated and discussed.

Design of solid composite propellants through modeling and numerical simulation

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Keywords: solid propellant; numerical simulation; ammonium perchlorate; ammonium nitrate.

Over the years, double base propellants have successfully fulfilled the requirements imposed by specific missions. However, the technological process of manufacturing this category of propellants exposes problems regarding supply chain management, but also of toxicity. This is why the new solid composite propellants have been developed, based on ammonium nitrate and ammonium perchlorate. The purpose of this paper is to determine, through modeling and numerical simulation, both the performance and ballistic characteristics of the newly heterogeneous propellants, by reference to the well-established solid double-base propellant. The influence of the burning surface was also highlighted, looking forward to succeed in achieving highest values of the parameters of the newly developed propellant.

An accelerated aging study of LLM-105 and its plastic bonded explosive

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Keywords: LLM-105; aging; characterization.

The high explosive 2,6-diamino-3,5-dinitropyrazine-1-oxide, LLM-105, is an energetic material with good performance and safety characteristics. This molecule has been widely reported on in the energetic materials community for nearly 30 years. However, there have been no comprehensive studies on understanding and characterizing its aging characteristics. Our investigations have focused on establishing a baselining for the LLM-105 and one plastic bonded explosive containing the molecule and evaluating the materials in accelerated aging tests to establish aging characteristics of the material. This contribution focuses on the safety, chemical, and thermal characteristics of the molecule and the selected formulation of such.

Tungsten and copper (II) oxide mixtures as gasless time-delay compositions for mining detonators

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Keywords: time delay compositions; detonators; solid state reactions; burn rate.

The widespread use of pyrotechnic compositions in time-delay detonators is the reason for research aimed at expanding knowledge of the kinetics of combustion of pyrotechnic mixtures. New compositions are being sought, the components of which would react with each other in the solid or liquid phase. Such a method of combustion would make the rate of combustion independent of the pressure inside the detonator. This paper presents the effect of the parameters of W/CuO mixtures on their rate of combustion. Depending on the quantitative composition and density of the mixture, the combustion rates were found in the range of 4.1 - 5.9 mm/s. The heat of combustion of the given composition in a wide range of quantitative composition was measured. The gas-free combustion mode of the proposed composition was proved using DTA and XRD. Determination of the qualitative composition of the combustion products allowed calculation of the adiabatic temperature of combustion.

Energetic material compatibility testing – what is it really telling us?

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Keywords: compatibility; HFC; DSC; propellant; nitrocellulose.

Research and development of new, exciting, energetic materials and associated formulations continues at pace. An important step in the development of a new munition is ensuring its safety throughout its life. Part of that process is to ensure that your energetic materials are chemically compatible with the other elements of the weapon system. The NATO standard, STANAG 4147, details the methodology behind chemical compatibility assessments, as related to munitions. Compatibility testing was conducted on M7 propellant and different inert contact materials using: Heat Flow Calorimetry (HFC), Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA). Analysis of these test results demonstrates the differences in compatibility assessments against each test method. HFC testing using different sample particle sizes was conducted and any influence on the compatibility assessments reported.

Explosive train modeling based on small scale tests

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Keywords: explosive train; energetic materials; combustion; detonation; initiation.

An energetic material (EM) can be initiated or detonated by an arrangement of EM placed together in a train by which the initial force from the stimulus is transmitted and intensified until it reaches and sets off the main acceptor. Specific design variables such as EM quantity, sensitivity, particle size, confinement type and thickness all affect the stimulus transfer process. Despite the critical uses of such initiation systems in defence applications, testing and understanding of such have been confined to empirical measurements to determine whether a proposed design is sufficiently reliable for the intended use. Modeling and simulation (M&S) can augment the testing process by reducing experimental iterations, expand the scope of study to include more variables and shed light on the observed outcome with a scientific understanding. Various initiator configurations are designed to study the effect of the aforementioned variables and small-scale tests are conducted to study the probability of initiation. Numerical models are developed to evaluate said variables in order to predict the response of the overall train, as well as to provide scientific reasoning for the predicted outcome based on fundamental principles. Zirconium potassium perchlorate (ZPP) is used as the igniting stimulus, to set off different amounts of receiving acceptor materials. Despite being widely used as the igniting propellant in an explosive train, its burning mechanism is not widely reported. In this work, the reaction model for ZPP is assumed to follow Vielle's law, and its parameters are calibrated and optimized based on measured combustion pressures from specially designed small scale tests. The calibrated burn model parameters act as inputs to the hydrodynamics model of an explosive train comprising of the ZPP stimulus, donor and acceptor explosives. With calibrated reaction models of the EMs, the response to different configurations of stimulus, acceptor and donor could be predicted. This methodology can be applied to study the burn models of EMs with little reported reaction mechanisms.

Formulation of energetic resins for additive manufacturing

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Keywords: 3D printing; resin formulation; energetic polymers.

3D printing offers enormous potential to produce on-demand complex propellant grain geometries, which are otherwise impossible with traditional manufacturing methods. This delivers opportunities for customizable burn rates. However, very few energetic materials can be 3D printed by the vat polymerisation method and display poor mechanical properties. This talk presents energetic resins formulated specifically for vat polymerisation.

Improved measurements of impact sensitivities of energetic materials

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Keywords: energetic materials; impact sensitivity; Bruceton method; confidence intervals; HMX.

Accurate estimation of impact sensitivity is crucial for safe production, handling, storage and transport of energetic materials. Indeed, molecular characteristics will affect sensitivity, and for solid materials, factors like particle size, lattice defects and morphology also play a role and make reproducibility difficult. As various synthesis and recrystallisation methods may lead to differences in crystal properties, it is important to determine the impact sensitivity whenever an energetic material is prepared. Of particular interest is the median h_{50}, namely the impact energy level at which there is a probability of 50% of an explosion occurring. This value has been shown to correlate with quantum chemical properties of the energetic material in question, providing insight into the underlying causes which govern sensitivity. However, in practical applications, it may be more important to estimate extreme values like the 99% quantile h_{99}. In addition to providing point estimates, we would like to derive confidence intervals to address their uncertainty. In this work, we cover the most common methods for constructing such confidence intervals (the delta method, Fieller's theorem and the likelihood-ratio test) and compare their performance on sensitivity data via simulations. Our experiments indicate that Fieller's theorem is the superior method, and we therefore use it to construct confidence intervals for h_{50} and h_{99} for cyclotetramethylene- tetranitramine (HMX), using new data. Based on our results, we formulate recommendations for researchers measuring sensitivities of synthesised molecules.

Minimisation of by-products and optimisation of the yield in the synthesis of BuNENA

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Keywords: BuNENA; flow chemistry; design of experiment.

The synthesis method of N-butylnitratoethylnitramine (BuNENA) and the formed by-products in this synthesis are well documented and available in patents and publications. Less information is available on how different reaction parameters effect the purity and yield in this reaction. This article describes the work of reaction parameter optimisation for the minimisation of by-products by the use of factorial design and flow chemistry. The following parameters were investigated: Temperature, residence time (would be called reaction time in a batch synthesis), and the ratio between the reagents. The study revealed that very high purity can be obtained, but that this effects the yield negatively. The so called sweet spot is defined not only by the reaction parameters, but also by the requirements on the component in a formulation. The work presented here shows that BuNENA can be produced in microreactors with high yield and purity.

Investigation of a new promising process for RDX and HMX synthesis via TRAT and TAT

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Keywords: energetic materials; hexogen; industrial production; octogen; synthesis.

Despite intensive research for possible replacements, RDX (hexahydro-1,3,5-trinitro-1,3,5-triazine) is still considered to be one of the most important energetic materials because of its economic and technical advantages. Due to the high demand for RDX, optimization of synthesis and development of new methods are of great interest to both academia and industry. Therefore, in this work, the synthesis of RDX via the intermediate TRAT (hexahydro-1,3,5-triacetyl-1,3,5-triazine) was investigated as a possible alternative industrial production method. In addition to the synthesis of TRAT starting from 1,3,5 trioxane, various feasible nitration methods from TRAT to RDX were also investigated. Moreover, the suitability for large-scale production, the comparison of already established methods and the feasibility of a flow process were investigated.

Nitrolysis of cellulose – an investigation of hydrolysis under nitration conditions

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Keywords: NC; nitrolysis; hydrolysis; nitration.

Nitrocellulose is industrially produced from cellulose by nitration in the presence of concentrated nitric and sulfuric acid. While sulfuric acid is known to catalyse hydrolysis of cellulose, the final chemical products of simultaneous nitration and hydrolysis (nitrolysis) are not fully characterised. Nitrolysis of cellulose has the potential to reduce the chain length and polydispersity of the resulting nitrocellulose producing more tunable homogeneous materials. Simultaeously it has the potential to produce nitrate-ester sugars, which are known to have an increased impact sensitivity,[1] compromising the safe handling of nitrocellulose. Here, the nitrolysis products of cellulose are studied via gel permeation chromatography, nuclear magnetic resonance and x-ray diffraction to characterise the changes and properties of nitrolysed cellulose.

Optimization of continuous method nitration of toluene by dinitrogen pentoxide/chloroform solution with using design of experiments (DoE) methods

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Keywords: selective nitration; dinitrogen pentoxide; design of experiment; TNT production.

In this paper was described selective nitration of toluene by solution of dinitrogen pentoxide in chloroform by continuous method. There was used Design of Experiment methods for optimization. Parameters of process were: temperature, time of residence in reactor, molar ratio toluene: dinitrogen pentoxide.

Energetic formulations of oxyhalide salts

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Keywords: oxyhalide salt; halogen.

Halogens are highly reactive and they and their oxides are often employed for their oxidizing power. We have previously reported the decomposition of iodates to form sufficient iodine and heat to be used as a biocide. In that study we found calcium iodate to be most effective. Now we compare three halogen oxy salts (EO_3^-, where E = Cl, Br, or I) in terms of their ability to produced molecular halogen and/or extremely high temperatures for complete destruction of biological agents or other materials. They are examined alone and with fuels.

Synthesis and reactivity of 5-hydrazino-3-nitro-1,2,4-triazole (HNT): an amphoteric energetic platform

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Keywords: nitrotriazole; energetic salts.

The first synthesis of 5-hydrazino-3-nitro-1,2,4-triazole (HNT) as a free base is described, from 5-bromo-3-nitro-1,2,4-triazole (BNT) in three steps. HNT exhibited amphoteric properties which were demonstrated through the synthesis of both cationic and anionic salts. Densities and enthalpies of formation of compounds 3-6 and 10 were measured and the respective P_CJ and D_CJ were calculated using these experimental data. Among the compounds derived from HNT, perchlorate 7 exhibits remarkable properties, with a high density of 1.95 and an outstanding detonation velocity (9505 m.s^{-1}) and pressure (419 GPa), thus surpassing RDX in performance.

Fluorinated binders for metal oxidation

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Keywords: fluorinated binder; cast curing; aluminum; heat of oxidation.

Fluorinated polymers serve as both oxidizer and binder in energetic formulations. Very few fluoropolymers exist that have functional groups such as hydroxyl that are suitable for curing and thus can be used as binders in castable or extrudable compositions. In this paper we report on the synthesis and characterization of novel cast curable fluoropolymers for binder applications. The potential of the fluorinated polymers to oxidize metal fuels is also demonstrated.

High resolution temporal and spatial studies into sympathetic reaction of commercial detonators: Initial studies

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Keywords: detonator; ouput; time-resolved.

Each year approximately 99% by mass of energetic material use takes place in the quarrying, mining, construction and petrochemical industries. One of the main commercial items used in these areas are detonators. Three principal factors determine the design of commercial detonators: reliability, safety and cost. In this paper we report an initial study using synchrotron radiation to produce high-resolution images of a sympathetic detonation between two commercially available detonators. Such events are a well-known hazard within the energetics community and can result in serious accidents in the transport and handing of such systems. This images clearly show the process of the sympathetic detonation in detail, allowing the detonation wave, compression of a granular barrier layer and the take over into the second detonator. These images were captured at the ESRF, ID19 beamline, using its newly established detonation chamber.

Parameter tunning in microfluidic flow-focusing droplet generators for tailored ADN emulsions

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Keywords: emulison; microfluidics; ADN.

Microfluidic systems allow highly monodisperse droplet formation for numerous lab-on-a-chip and chemical synthesis applications, while also offering a wide range of adjustable droplet sizes. This benefit was used in this work to design the shape of ammonium dinitramide (ADN) droplets, respectively crystals. ADN is a promising green oxidizer that can replace ammonium perchlorate in solid rocket propellants. To achieve high packing density, it is necessary to utilize ADN as spherical crystalline particles with defined size. A microfluidic emulsion crystallization process was developed. Droplet formation regimes were identified as a function of the capillary number and described in terms of droplet size and droplet size distribution.

Synthesis of CL-20 by palladium free route by using cyclopropylamine based cage structure

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Keywords: CL-20; cage structure; nitration; explosive; cyclopropylamine; palladium-free route.

Cl-20 is a well-known high energy material used worldwide. The preparation od CL-20 require a caged precursor made by a reaction between a primary amine and Glyoxal. The caged structure was reported with Benzylamine. The CL-20 has been synthesized industrially by using hexabenzylhexaazaisowurtzitane (HBIW). Although, the conversion of HBIW to hexanitro-hexaazaisowurtzitane (HNIW or CL-20) involves multiple steps, namely, cleavage of the benzyl groups using Pd/C catalyst, in-situ acylation with acetic anhydride, finally nitration, and the overall product yield was around 45%. Therefore, researchers have been keen on replacing benzylamine in order to avoid the expensive and sensitive step of catalytic hydrogenolysis of the cage structure in the synthesis of CL-20. The caged structures are possible with few of the amines like substituted and unsubstituted Benzylamine, propylamine, thienylamine, pyridylamine, furfurylamine, naphthylamine, cinnamylamine, allylamine and propargylamine. Unfortunately, the isolation and purification of resulting products was found to be cumbersome. We have undertaken a synthetic route study on a reaction between glyoxal and using primary amines such as cyclopropyl amine. Thus prepared cage structure was hexacyclopropylhexaazaisowurtzitane (HCPIW). The formation of diimine intermediates is stable and it can be isolated in case of aliphatic primary amine. There is evidence by HRMS data that the mechanism undergoes by the formation of diimine and cyclotrimerization takes place to form cage compound (HCPIW). This cage structure was found to be converted to CL-20 in a single step by nitration. Thus we are able synthesize CL-20 by palladium free route.

Synthesis, characterization and comparison of differentially bridged nitraminotriazoles and their energetic salts

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Keywords: energetic materials; triazole; synthesis; characterization; bridged azoles.

In this work, two new bridged nitraminotriazoles were synthesized with oxapropyl and nitrazapropyl as bridging moieties. Furthermore, several energetic salts were obtained based on the two new compounds, as well as the literature known hydrazonemethyl bridged nitraminotriazole. All new compounds were fully characterized by NMR, IR spectroscopy, elemental analysis as well as differential thermal analysis. The sensitivity towards friction and impact were determined according to BAM standard technics and the energetic properties were calculated by using the EXPLO5 computer code. The neutral compounds as well as the various salts were compared in terms of physiochemical properties and detonation performance to each other and to the commonly used secondary explosive RDX.

Adding machine learning approaches to RoseBoom2.3

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Keywords: prediction of performance; computer program.

When looking through literature, various methods are used to predict the properites of energetic materials, often with questionable precision, for key values such as the enthalpy of formation deviating by upto 200 kJ/mol. In this article artificial intelligence is used to improve the precision of values predicted by RoseBoom2.3. The programme uses values harvested from the literature and structural recognition, to convert strcuture into a machine readable format. This allows values to be calculated in a short period of time, to obtain a consistent basis for such values which is important when comparing different molecules.

Accelerated aging characteristics of AP/HTPB based solid composite propellants and service life determination models

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Keywords: accelerated aging; composite solid propellant; service life determination model.

The properties of composite solid propellants change gradually due to interactions with the environment, propellant components, and other parts of the munition system. The accelerated aging study is vital to reveal the behavior of propellant properties over time and to determine essential properties. This study investigated the physical, chemical, ballistic, and mechanical properties of AP/HTPB-based propellant formulation at three different accelerated aging temperatures. The changes in mechanical and viscoelastic properties with aging were investigated. In addition, Arrhenius-based pseudo-first-order storage life models are compared with a model that reflects the competitive aging mechanism more accurately.

Effects of addition of opacifiers on the laser ignition of NC-GAP propellant

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Keywords: double base propellants; laser ignition; carbon black; berliner blue.

Laser initiation has received considerable attention as a method for igniting energetic materials, because it allows precise control of the amount of energy, pulse duration, and the area of exposure, which enables better control of the ignition process and consequently improves safety. It is often challenging to achieve sustained ignition in solid propellants due to a lack of optical absorptivity at convenient wavelengths. This means that the use of an opacifier to decrease reflectivity and increase radiative absorption at the propellant surface is necessary. Carbon Black (CB) and Berliner Blue (BB) were used as opacifiers in different proportions in film samples of double base propellants made of nitrocellulose (NC) plasticized with glycidyl azide polymer (GAP), and the response of the samples to a laser was tested. In addition, thermogravimetric analysis (TGA), and FT-IR spectroscopy of the infrared region were investigated, and the sensitivities to external stimuli (friction, impact) were also determined. Minimal addition of CB (1% mass) proved effective in making the propellant laser reactive, while only minimally affecting the sensitivities and thermal characteristics of the sample, compared to the sample without opacifier additives.

Combustion analysis of the quaternary first fire mixture

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Keywords: first fire; quaternary mixture; barium peroxide; barium nitrate; magnesium; combustion residue.

This paper investigates the residue after the combustion of first fire mixture based on barium peroxide, barium nitrate, magnesium and phenol formaldehyde resin iditol as a binder. Residue components were determined using reaction stoichiometric, EXPLO5 computation, and SEM/EDS analysis.

2-azidoethyl-tetrazole as a ligand for laser-ignitable energetic materials

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Keywords: energetic coordination compounds; primary explosives; sensitivities; laser ignitability.

The energetic 1-azidoethyl-tetrazole (AET) has already been proven to function as a ligand in several energetic coordination compounds (ECCs). This work seeks to introduce the 2-azidoethyl-tetrazole (2-AET) isomer, which has so far not been reported in literature, as a powerful ligand for ECCs with potential application as laser ignitable primary explosives and compare its value to the AET ligand. Therefore, ECCs that carry the 2-AET ligand were produced and characterized concerning their sensitivities, thermal stability, ignitability by laser irradiation, vibrational spectroscopy and by low temperature XRD.

Development of an azidoethyl-transfer reaction protocol for azoles

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Keywords: synthesis; azoles; alkyl transfer; azides.

The azide functional group is fundamental for many areas of chemistry, including energetic materials, drugs, as well as for organic synthesis e.g. in click chemistry. In recent years, specifically organic azides have gained a lot of interest in the field of HEDMs as possible energetic plasticizers, binders, additives, or high explosives. The availability of organic azides often relies on either halide to azide exchange reactions or on direct introduction of an azide containing alkyl chain. These reactions are highly dependent on the starting material and often cannot be universally used. The use of customizable transfer reagents increases the availability and introduces new reaction pathways. Many azidomethyl derivatives of prominent heterocycles have been extensively studied, while azidoethyl containing compounds are far less available. Therefore, 2- azidoethyl 4 toluenesulfonate was prepared as an azidoethyl-transfer-reagent and reacted with the five-membered azoles imidazole, pyrazole, 1,2,3-triazole, 1,2,4-triazole and tetrazole. A reaction protocol that is applicable for all common azoles and that is expandable to other transfer reagents was developed and optimized. The transfer reagent as well as the products of the azidoethyl transfer were characterized through multinuclear NMR and IR spectroscopy, and tested for their thermal behavior.

Characterization of TATP as a donor charge in a detonation train

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Keywords: tertiary explosives; TATP; detonation; booster.

Tertiary explosives are characterized by their low shock sensitivity and their strong nonideal character. They are often widely available on the market without or with limited restrictions. Their use in conjunction with homemade explosives (HME) is of great concern for counterterrorism actors, especially if they can be detonated with a limited quantity of HME as a booster charge. It is however difficult to assess this issue because the detonation properties of the donor charge and the shock sensitivity of the acceptor charge are mostly not documented, but also because the non-ideal character and the low shock sensitivity of the tertiary explosives imply the use of very large donor and acceptor charges. Moreover, the synthesis, shaping, and safe handling of HME charges at the kilogram scale is made extremely complex by the very high sensitivities of most HMEs. Most of the studies on HMEs are furthermore focused on synthesis, sensitivity, and performances, but not on their detonation properties as a donor charge. In this work, we study the detonation properties of triacetone triperoxide (3,3,6,6,9,9-hexamethyl-1,2,4,5,7,8-hexoxonane, TATP) as a donor charge in a detonation train. A loose density of 0.5 g/cmş was selected to reproduce real operational conditions. A teleoperated process was developed to load TATP, synthesized in 5 g batches, into charges of hundreds of grams in a safe and reproducible manner. A representative charge geometry was selected based on preliminary testing. The detonation velocities at different densities were experimentally determined and compared with results obtained from thermodynamical calculations to evaluate the non-ideal behavior of the charges. The potential of different simulants to substitute TATP is discussed.

Calculated performance parameters of detonated nitrocellulose-based propellants

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Keywords: detonation; propellant; nitrocellulose.

Nitrocellulose-based propellants are the most widely used in modern ammunition, rockets and missiles. Knowledge on their detonation performance can be very valuable in safety and other possible considerations. There are many types of propellants that have different chemical composition. Some are mainly with nitrocellulose only, but others can have other energetic components, such as nitroglycerin, dinitrotoluene etc. Their grain shapes and dimensions significantly differ also, which can have significant influence on their detonation performance also. Calculated detonation performance parameters for different nitrocellulose-based propellants are presented in this paper. Modern types of propellants for different weapon systems were considered. Appropriate numerical models of detonation were used to calculate different performance parameters. Calculation results were compared with experimental data, where possible.

Energetic properties of ZrW2 and HfW2 under impact

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Keywords: reactive structure material; ZrW2; HfW2; drop hammer; impact-initiated energy release.

Interest in reactive structure materials (RSMs) as potential candidates for increasing the overall performance of weapon systems is growing rapidly. RSMs are capable of dramatically increasing the total amount of energy that can be released. Two promising materials that can be used as RSMs are ZrW_2 and HfW_2. Compacted powder samples of ZrW_2 and HfW_2 were prepared and investigated for their energy release properties. For this purpose, W and Zr or Hf pieces were melted in stoichiometric amounts in an electric arc melting station. The resulting samples were milled in a mortar mill into fine powders and subsequently compacted in an uniaxial press. Energetic properties were examined by BAM drop hammer tests. Fragments were captured and analyzed to gain insights into the initiation mechanism.

Applying machine learning techniques to balance performance and stability of high energy density materials

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Keywords: impact sensitivity; machine learning; electrostatic potential; HOMO-LUMO gap; dipole moment; doorway modes; Fukui indices descriptors.

The long-standing stability-performance contradiction issue of high energy materials (HEMs) is of extremely complex and multi-parameter nature. Herein, machine learning has been employed to fit a possible relationship between the selected descriptors and the impact sensitivity. Four models, namely Extra-Trees regressor, Gradient Boosting for regression, Random Forest and Support Vector Regression, were respectively trained and evaluated by stratified sampling and 4-fold cross-validation methods. Among them, the Support Vector Regression model produced the best scoring metrics in predicting the impact sensitivity of HEMs. Feature importance analysis was conducted to obtain data-driven insight into the causality of the performance-stability contradiction and delivered the optimal range of key features for a more efficient rational design of advanced HEMs.

Blasting properties of low-density emulsion based mixtures

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Keywords: emulsion based explosives; velocity of detonation; work ability.

Emulsion explosives are commonly used for civil purpose blasting. In order to decrease impact effect on surrounding rock mass, it is possible to reduce detonation pressure and borehole pressure with reducing of density of proposed explosive emulsion based mixtures. In that case reduction of the velocity of detonation is also achieved. In focused testing, emulsion matrix has been sensitized with expanded polystyrene. Mixtures with different portion of EPS have been prepared and blasted in rock bore holes. According to measured velocity of detonation values, relationship with density and work ability has been determined.

Synthesis and characterization of high energetic materials based on 1,2,3-triazoles and 1,3,4-oxadiazoles

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Keywords: triazole; carbonyl azide; oxadiazole.

1,2,3-Triazoles are favorable backbones in energetic materials, they provide a high heat of formation; and are easily accessible through 1,3-dipolar cycloaddition of an alkyne with an azide. In this work the 4-and 5- positions of 1,2,3-triazole was functionalized with 1,3,4-oxadiazoles and acyl azides in a straightforward synthesis. The compounds were analyzed with multinuclear NMR and IR spectroscopy, elemental analysis, X-ray diffraction and the thermal stabilities were measured using DTA. The heat of formation was calculated on CBS-4M level of theory and the explosive parameters were computed using the EXPLO5 code. The sensitivities towards friction and impact were measured by applying the BAM procedure.

Controlled synthesis of star-shaped hydroxyl-terminated polybutadiene

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Keywords: binders; model polymers; HTPB.

PHydroxyl-terminated polybutadiene (HTPB) is an essential prepolymer in the preparation of binders for fuels in solid rocket motors. Traditionally, HTPB is prepared via free-radical polymerization of butadiene, resulting in broad and uncontrolled molar mass distributions and polymer architectures. Chief among the non-uniformity of the resulting prepolymers is the number of hydroxyl groups present within a single polymer chain. This has deleterious effects given that curing with isocyanates to form the final binder material requires reaction with the hydroxyl groups of HTPB. The amount of hydroxyls therefore has significant impact on the rate of increase in viscosity during processing and energy obtained from the binder itself. Accordingly, it is unclear what the optimal amount of hydroxyls is for HTPB use in binders. This project seeks to prepare a series of star-shaped HTPB polymers via reversible addition-fragmentation chain-transfer (RAFT) polymerization. RAFT is a well-established polymerization technique that yields polymers of narrow molar mass distribution and with controlled architecture. Therefore, the polymers produced herein will allow for systematic investigation into the effect of hydroxyl group content in HTPB based binders. Presented is the initial investigation into this field, beginning with the synthesis of necessary chain-transfer agents for the RAFT polymerizations.

Effects of mechanical impact on PBX disks investigated by IR and Raman spectroscopy

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Keywords: PBX; impact tests; damage analysis; spectroscopy.

During firing of ammunition, embedded high explosives charges are exposed to significant setback loads, e. g. in a tank gun. To simulate loading scenarios and analyze resultant damages in explosive charges, plastic bonded explosive (PBX) disks of HMX in cured hydroxyl-terminated polybutadiene binder were manufactured, exposed to projectile impacts in so-called safety threshold tests (STT), and the PBX disks were analyzed before and after the impact tests. The analysis includes friction and impact sensitivity tests, dynamic mechanical analysis (DMA), X-ray diffraction (XRD), nano computer tomography, and spectroscopy. Detailed results obtained by DMA were reported during the last NTREM. Now results of IR and Raman spectroscopic investigations are presented. The evaluation revealed significant changes of the spectra after STT loading, such as band broadening and shifts, particularly of bending and stretching vibrations of the nitramine groups of HMX. The results are discussed in context of crystal inhomogeneities and first reaction steps of the HMX.

Solubility determination and recrystallization studies of guanidinium 5,5'-azotetrazolate

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Keywords: solubility; crystallization; guanidium azotetrazolate.

The purpose was to determine the solubility data of guanidinium 5,5'-azotetrazolate (GAzT) in various pure solvents including methanol, ethanol, acetone, acetonitrile, ethyl acetate, 1,4-dioxane, N,N-dimethylformamide (DMF), and Dimethyl sulfoxide (DMSO) at temperatures T = 25řC, 50řC and pressure P = 1 atm. Solubility data of guanidinium 5,5'- azotetrazolate showed the maximum value in DMSO, followed by water and DMF. Recrystallization experiments were conducted by mixing GAzT in various solvents with selected anti-solvents. The morphology and structure of the produced crystals were analyzed using optical microscopy.

High burning rates propellants based on GAP

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Keywords: high burning rate; plasticizer; catalyst; GAP.

The aim of the research was to create a wide range of solid rocket propellants with heightened energy and burning rate. All the propellants were tested to determine their properties. As the binder, either HTPB or GAP were added. The oxidizer used was ammonium perchlorate or an ammonium perchlorate and high energy oxidizer such as HMX blend. Either ADO or TMETN were the plasticizers. The propellants were examined to determine their density, toughness, sensitivity to friction and their burning rate. It was proven that the components and the ratios of them in the propellant's composition make a great difference in the propellant's properties.

Performance of 3D printed shaped-charge liners

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Keywords: shaped charge; shaped-charge liner; 3D printing; metal infused PLA.

The development of additive manufacturing has led to a point where it is possible to 3D print objects from a wide variety of materials. Some of those materials include PLA plastic filament filled with metallic powders, such as copper, steel, and bronze. The printed object weighs more, and if polished it can look as if it was made entirely from metal. The commercial availability of 3D printing makes it easy to use it for prototyping of improvised components capable of enhancing the effects of explosives. This work is about the performance of liners for shaped charges made by 3D printing with copper filled filament. Two geometries were studied, both in two different diameters and tested at two different stand-off distances from the target. The explosive used was a cast mixture of TNT/HMX in 40/60 weight percent. The results show a perforating depth of up to 54mm in steel.

Application of calorimetry to estimate the thermal performance of thermobaric explosives

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Keywords: calorimetry; thermobaric explosive; thermal effect; metal powders; thermodynamic code.

Reactive metal powders are often added as a fuel component to thermobaric explosive compositions in order to enhance the total heat released during the post-detonation combustion in the detonation fireball. These metals are selected regarding their heat of combustion, but also taking care of ease of ignition and safety during the preparation of the mixtures. For the thermobaric explosives, it is crucial to perform adequate quantification of their performance, not only regarding the detonation parameters but also regarding the blast effect and the developed heat. This research considers the application of calorimetry on small samples of thermobaric explosive mixtures containing different metal powders. The energetic potential for the selected thermobarics was determined in an isoperibolic calorimeter and the obtained results were compared to calculated values obtained in thermodynamic code for isochoric combustion of the observed compositions. IR camera was applied to track the thermal output during the open air combustion of the prepared thermobaric mixtures.

On the effects influencing calorimetric measurement of the heat of explosion

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Keywords: bomb calorimeter; single-base propellant; heat of explosion.

The explosion heat is one of the key parameters of gun and rocket propellants. It is determined using bomb combustion calorimetry in an inert atmosphere. The amount of heat is determined from the temperature increase of water bath in which the bomb is submerged during the test. Although the method is relatively simple and straightforward, there are some parameters that may significantly affect the measurement results in some cases. Calorimetric measurements were performed using single-base propellant samples at various sample weights, bomb volumes, and bomb atmospheres. The experimental results were compared with the calculated values obtained from the EXPLO5 thermochemical code. Errors recorded under suboptimal measurement conditions were quantified.

Thermal and ballistic properties of ZPP based priming mixtures

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Keywords: ZPP; additives; priming mixture; ballistics; electric initiator.

The ballistic properties of ZPP and ZPP with additives Al2O3, MnO2, Fe2O3 and CuO were studied in conditions of electric initiator (squib) by closed bomb test. The heats of combustion of all compositions were measured on an adiabatic calorimeter. Measured data were used in REAL software to obtain reaction equations and reaction temperatures. The additives were shown to have a significant impact on the ballistic and thermal properties of the mixture.

Small-scale detonation velocity measurements using fiber optic probe

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Keywords: plastic optical fiber; failure diameter; detonation; semtex.

The paper focuses on detonation velocity measurement of small diameter charges of Semtex 1A. A series of unconfined cylindrical and conical charges with a diameter of 1-5 mm was tested. Detonation velocity measurements were made using the perforated fiber optic probe technique which utilizes plastic optical fiber with a linear array of small holes drilled into the core. The utility of this technique in failure diameter measurements has been demonstrated. The diameter effect in the explosive was revealed and quantified in the region near the failure diameter. The detonation velocities adequately complement the previously measured results for larger charge diameters. The data may be helpful in the parametrization of non-ideal detonation models in thermochemical calculation codes.

Explosion parameters of air dispersed nitrocellulose ignited by exploding wire

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Keywords: nitrocellulose; dust explosion; exploding wire.

Nitrocellulose is flammable compound produced by cellulose nitration in large scale. Dry nitrocellulose is a highly flammable fibrous material. On burning, it gives a yellow flame; in larger quantities, it can generate a sensitive heat wave. Nitrocellulose may detonate or burn upon certain conditions. The article present the combustion parameters of air dispersed dry nitrocellulose (marked E24) in the KV-150M2-UIBE explosion chamber at the concentrations of 60 - 1000 g.m^{-3}. A typical diameter of nitrocellulose sample fibres was 20 - 100 um and length up to 10 mm. Nitrogen content of the nitrocellulose was 12.55%. Exploding wire was used for ignition of nitrocellulose sample. Exploding wire is a local igniter. It consists of a capacitor (capacity 13000 uF @ 400 V) and kanthal resistance wire with a length of 2x2cm. The igniter releases 800 J of energy. It was found that with the increasing value of the concentration of nitrocellulose, the value of the explosion pressure P_*max* and also the explosion constant K_*st* increases.

Investigation of 3,5-diamino-1,2,4-oxadiazole as a precursor for energetic salts

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Keywords: precursor; 3,5-diamino-1,2,4-oxadiazole; hydrochloride.

1,2,4-Oxadiazole is an attractive backbone for energetic materials as it shows a positive impact on the oxygen balance compared to other heterocycles like imidazole or triazole. The suitability of 1,2,4-oxadiazole as a cation in energetic salts should be evaluated, as ionic compounds are known for high densities and low vapor pressure. 3,5-Diamino-1,2,4-oxadiazole (AOA) as a starting material can be easily synthesized from sodium dicyanamide and hydroxylammonium chloride. Despite indications in the literature to be acid sensitive, AOA hydrochloride was successfully synthesized. To the best of our knowledge, this is the first report of an AOA-based salt. The synthesized compound was characterized by NMR, IR spectroscopy, Raman spectroscopy, ion chromatography and thermal analysis.

Effect of tetrazene preparation conditions on its powder characteristics

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Keywords: tetrazene; characterization; bulk density; flowability; primary explosive.

The effect of tetrazene preparation conditions on its processing and sensitivity characteristics were studied. In industrial technology, tetrazene is prepared by reacting aminoguanidine sulphate or bicarbonate with sodium nitrite under weakly acidic conditions. The effect of changing the aminoguanidine starting material, reactant concentration and temperature of the reaction mixture on the powder characteristics of the prepared tetrazene was studied. The salts of aminoguanidine used were selected on the basis of their potential applicability in industrial technology, namely sulfate, chloride, nitrate and in situ carbonateprepared salts such as acetate, citrate, methanesulfonate and phosphate. The extent of the effect of these changes was assessed using bulk material characteristics (bulk density, angle of repose), particle morphology and granulometry.

Experimental vapor pressures of the commonly used plasticizer TMETN via transpiration method supported by quantitative chromatography

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Keywords: energetic material; glycol nitrate; transpiration method; vapor pressure; heat capacity.

Trimethylolethane trinitrate (TMETN) is a widely used additive for propellant mixtures. It is utilized in some solid propellants and smokeless powders as a plasticizer. Although a facile synthesis makes this substance widely available, no thermodynamic data exist regarding the volatility and the heat capacity. This work fills this literature gap by using the sapphire temperature jump method via differential scanning calorimetry for the heat capacity determination, as well as by using the transpiration method for the vapor pressure measurements.

Synthesis and analysis green pyrotechnic compositions

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Keywords: greening; pyrotechnic compositions; preparing; testing.

The design of a new formulation of ignition pyrotechnic composition will reduce the environmental burden and at the same time improve the working environment in the production and processing of pyrotechnic compositions. The proposed formulation meets current regulations for the use and handling of chemicals and complies with all safety and environmental regulations. It does not contain hazardous chemicals, which will also fulfil the conditions for innovative products and materials, increasing the safety of workers in the production, handling and subsequent use of such a "REACH compliant" ignition pyrotechnic composition.

Prediction of the enthalpy of formation by density functional theory calculations

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Keywords: enthalpies of formation; DTF calculation; compound Gaussian methods; enthalpies of sublimation; enthalpies of vaporization.

Enthalpies of formation (EoF) are important quantities in the determination of the performance data of explosive materials. Not always they are available. Several attempt and procedures exist to calculate them. There are structure-property correlation methods, additivity methods and quantum mechanical methods. For the prediction of the standard enthalpies of formation (EoF) of organic compounds, in our case for energetic materials and their components, semi-empirical computational methods based on quantum-mechanical (QM) methods were selected to calculate these values with sufficient accuracy. For the QM calculations, we have used the program suite Gaussian16 Rev. C.1.1 from company Gaussian^{TM} Inc [1]. The first step is the calculation of the standard enthalpy of formation in the gas phase. Two of many methods are to calculate the EoF via the enthalpies of reaction: (1) from elements to molecule; (2) atomization, from molecule to elements. For both methods, correction terms were developed: for (1) see Politzer [2] and for (2) see Rice [3, 4]. Further, the so-called compound (composite or multi-level) methods as CBS-QB3, G4, G4-MP2, W1-BD from Gaussian^{TM} Inc [1] are used for this purpose, which have higher accuracy than the normal density functional theory (DFT) -methods used by Politzer and Rice [2-4]. The second step is to get the enthalpies of formation of the condensed phases starting from the gas data. For this the enthalpy of vaporization must be substracted in case of a liquid and the enthalpy of sublimation in case of a solid, always at standard conditions. To obtain these data two empirical formulas are given to calculate them on the base of the electrostatic potential and the molecular surface, whereby the software given in [5] can be used to get the necessary parameters. Rice has adopted the Politzer method but used another set of molecules to determine the empirical fit parameters. Mainly CHNO molecules are of interest, but possibilities exist to include the elements S, P, F, Cl, and some others can be considered as Na, Mg, Al, Si. Examples on DPA and its nitrated products are presented, and the data are compared to experimentally and to a structure-property correlation method determined values of EoF based on molecular descriptors.

Attractive nitramines/polyaniline composite crystals via co-agglomeration

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Keywords: coagglomeration; impact sensitivity; nitramines; polyaniline; thermal decomposition.

Co-agglomerated microcrystals(CACs) of attractive nitramines (NAs) RDX, HMX, BCHMX and CL20 coated with electrically conductive polyaniline (PANi) were prepared using Co-agglomeration method, in which PANi forms a charge transfer complex with these polynitro compounds. Based on the thermal analysis study, the activation energies of the decomposition processes of pure and modified PANi-NAs are determined using the Kissinger method, and thermal decomposition processes are discussed. Except for RDX/PANi CACs, all other CACs show higher activation energies for decomposition compared to their pure NAs counterparts. The relations between the activation energies of thermal decomposition, on the one hand, and the squares of the detonation velocities, enthalpies of formation and impact sensitivities of the studied EMs, on the other hand, are specified. Also described are the relationships between the low-temperature heat of decomposition from DSC of the studied EMs and their enthalpy of formation as well as impact sensitivity. Based on the obtained results, the exceptional desensitization of BCHMX by coating its crystals with polyaniline is pointed out which is also discussed.

2D numerical simulation of two metallic concentric tubes explosively-driven

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Keywords: Gurney velocity; concentric tubes.

In this numerical study was defined and analyzed a cylindrical configuration containing two concentric steel tubes, not in contact, filled with Composition B in both annular and central space. As a reference, a classic metal tube/explosive fill configuration was defined, having the same exterior diameter and the same metal/explosive ratio as the studied configuration. The models were built and run in AUTODYN 2D software (planar symmetry option). The analysis was focused on the Gurney velocity able to be reach by the two tubes. The charge detonation was set in two different hypotheses: 1) central charge and annular charge detonate simultaneous and 2) central charge detonates initially while annular charge suffers a sympathetic detonation. The results are slightly different for these two scenarios, but in both the exterior tube reach a velocity similar to that obtain in the reference simulation while the interior tube reach a consistently lower velocity.

Some observations on the role of scientific information in Poland – results of a survey conducted among researchers working with explosives

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Keywords: survey; scientific information; scientific journal.

Results of a survey conducted among participants of the IPOEX2022 conference (June 2022, Poland) and readers of Central European Journal of Energetic Materials are discussed. Data of 31 researchers working with explosives, and taking part in the survey, i.e. their education level (student, engineer, M.Sc., Ph.D or professor) and the both, the period (<3, 3-10, 11-20 and >20 years) and the place (university, research institute and production facility (> 50 employees)) of their scientific activity, were the basis of the analyzis. The survey was focused on the number and the kind of collected data sources (papers, books, paper/electronic version, etc.), on the role of scientific information in their's research work and on the kind of preferred sources of scientific information. Also their assessments what proves the informational value for readers of both, a scientific journal and a paper, were collected in the survey.

Development of a new screening technique for burning rate modification assessment

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Keywords: ballistic modifiers; closed vessel; ammonium perchlorate.

In order to develop a new and faster screening technique to determine the suitability of ballistic modifiers a testing closed vessel was used. A mixture of ammonium perchlorate and burning rate modifiers was used for these tests. The prepared samples were measured as powder material. To compare efficiency of each modifier used a pressure-time profile and pressure rate was determined. Catalyst that, accelerate the burning rate of ammonium perchlorate was used to verify reliability of the method. In addition, new burning rate modifiers were also used and some were found to be very promising.

Lithium tetrazole salts as green colorants in pyrotechnical formulations

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Keywords: aminotetrazole; flares; lithium salts; red pyrotechnic colorants; strobes.

Due to the negative effects of chlorinated components and strontium on human health and the environment in red-burning pyrotechnics, research int "green" substitutes has been increasing in recent years. One option to address these problems is the use of lithium 5-aminotetrazolate and dilithium 5,5'-bistetrazolate dihydrate as the respective colorant. Lithium has so far been considered harmless to human health. For this reason, various lithium salts based on nitrogen-rich organic compounds were used in pyrotechnical mixtures and their performance was evaluated in terms of burning time, dominant wavelength, spectral purity, light intensity and frequency. Furthermore, the sensitivities of the prepared formulations towards impact and friction were determined according to BAM standards.

Evaluation of input parameters for the non-ideal detonation model of emulsion explosives

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Keywords: emulsion explosives; non-ideal detonation; Wood and Kirkwood theory; EXPLO5 code.

Emulsion explosives exhibit non-ideal detonation behaviour. The degree of their nonideality depends mostly on their composition and density (i.e., porosity), which in turn is a function of amount of glass-microspheres added. Variation in composition results in a significant difference in the detonation properties. This presents an additional difficulty for numerical modelling of detonation of emulsion explosives since the input parameters for the modeling (such are reaction rate, equation of state of unreacted explosive, etc.) differ for each composition and density. In this paper we present the results of calibration of the constants in pressure-dependent rate model incorporate in the Wood-Kirkwood detonation model. The constants are determined for several low-density emulsion explosives which contain up to 50% glass micro-balloons, in such a way that they reproduce the experimental detonation velocities-charge diameters data. It was shown that pressure-dependent reaction rate model and the rate constants obtained in this study, can satisfactorily reproduce experimental detonation velocity-charge diameter for unconfined charges having densities in the range 0.5 to 1 g/cm^3.

Initial attempts in laser acceleration of thin metal plates

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Keywords: pulse laser; flyer; laser acceleration; photonic doppler velocimetry; metal foil.

The research of the explosive's initiation mechanism is part of the energetic materials engineer's task. Of many ways, the explosive can be initiated by a fast-moving thin metal plate, a flyer. The flyer is usually generated with another explosive or electric discharge; however, it can also be formed by laser ablation of the metal plate. For the laser ablation we used the Nd:YAG 532 nm nanosecond laser. In this work, we are showing the initial results of single-layer flyers generation. We tested aluminium foils in the form of a tape. The evaluation was performed in combination with photonic Doppler velocimetry (PDV). Obtained velocity proves the possibility of accelerating metal foils beyond 1 km/s using energy slightly over 100 mJ. The work provides the necessary basics for future work on the initiation by laser-driven foil impact.

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