Abstracts of the 26th Seminar on

New Trends in Research of Energetic Materials

Pardubice, April 17–19, 2024

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

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Held at the University of Pardubice

Pardubice, Czech Republic
April 17–19, 2024

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 into a well-established international event. Although 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 relationships with colleagues from countries all over the world.

The 26th 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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- SSE Explo, Czech Republic.

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 11th, 2024 Jiri Pachman

Synthesis, characterisation and energetic performance of a new copper complex based on 3,4,5-trinitro-1H-pyrazole

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Keywords: initiator; pyrotechnic; 3,4,5-trinitro-1H-pyrazole; ammonium copper (tetrakis) trinitropyrazolate [NH4)2[Cu(TNP)4].

The design of both initiators and pyrotechnics that are more environmentally benign ("green") relies on the use of nitrogen- or oxygen-rich materials that act as efficient oxidizing agents to reduce formation of particulates, together with less toxic metals such as copper. Herein, we report the synthesis and characterization of a new copper complex based on the trinitropyrazolate (TNP^-) ligand - ammonium copper (tetrakis)trinitropyrazolate [(NH4+)2CuII(TNP-)4], which displays remarkable thermal stability, combined with a high energy output. It is therefore a promising candidate to

Detonation simulant of TATP as a donor charges in a detonation train

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Keywords: TATP; tertiary explosives; detonation; booster; simulants.

Dual-use substances or those used to synthesize known homemade explosives (HME) are subject to strict controls. However, tertiary explosives are typically not classified as explosives under international regulations due to their exceptionally low shock sensitivity and non-ideal characteristics. Their ready availability raises significant concerns for counter-terrorism efforts, especially when they are used in conjunction with relatively small charges of HME as booster charges. Assessing this issue is challenging because data on the detonation properties of the donor charge and the shock sensitivity of the acceptor charge are often lacking. Most studies on HMEs primarily focus on synthesis, sensitivity, and overall performance, while the examination of tertiary explosives necessitates the use of large donor and acceptor charges. Due to the very high sensitivity of most HMEs, the synthesis, shaping and safe handling of kilogram-scale HME charges are moreover extremely complex. To circumvent these challenges, this work aims to develop simulation booster charges composed of diluted secondary explosives with detonation properties closely resembling those of the HMEs under consideration, such as triacetone triperoxide (TATP), while maintaining the sensitivities of secondary explosives. First, we investigated the detonation properties of TATP as donor charges in a detonation train. We developed a teleoperated pneumatic system to safely and reproducibly shape TATP charges at realistic densities, utilizing confined charges to approach infinite-diameter properties closely. The detonation pressure and shock adiabate of the detonation products were experimentally determined based on measured attenuated shock velocity in inert acceptors, and the experimental detonation products' isentrope was derived from cylinder expansion test results. These experimental findings were then compared to thermodynamic code calculations to assess the non-ideal behavior of TATP charges at 0.4 g/cm3. Subsequently, we conducted a similar characterization of proposed simulants, which replicate the detonation properties of TATP, particularly at a loose density of 0.5 g/cm3, as a basis for reproducing its detonation characteristics as a donor charge for safety margins. These simulants included Urea hydrogen peroxide (UHP) and diluted Nitro Methane. Their results were then compared to those predicted for TATP at 0.5 g/cm3 density. These candidates showed satisfactory agreement in the reflected Hugoniot of the detonation gases and the isentrope of the detonation products, suggesting them as promising simulants for TATP. This comprehensive study offers valuable insights into the potential use of these simulants as detonation surrogates for HMEs when employed as booster charges for tertiary explosives.

Synthesis of graphene oxide/nano-silica composite and its application for decontamination of 2,4-dinitroaniline from water

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Keywords: reduced graphene oxide; silica nanocomposite; removal of explosive; 2,4-dinitroaniline.

Large scale manufacturing and processing of high energy materials for application in defense, aviation and space programs generate huge amount of explosive waste, which leads to the deterioration of our natural resources like water and soil. Therefore, concrete steps must be taken for treatment of explosive waste. Here, thermally reduced graphene oxide/nano-silica (rGO/nSiO2) composite was synthesized for its application for removal one of the explosive, 2,4-dinitroaniline (DNA). The synthesized nano-composites were characterized for morphological (Scanning Electron Microscope & Transmission electron microscope), physical (X-Ray Diffraction), chemical (Fourier Transform Infrared & Raman Spectroscopy) and thermo-gravimetric analysis. The morphological characterization of the nano-composites confirmed uniformed distribution of nSiO2 in a size range of 9-14 nm on the surface of reduced graphene oxide. Physical and chemical characterization illustrated crystallinity, chemical and thermal behavior of the nano-composite. Its efficiency towards removal of explosive (2, 4-DNA) was analyzed by UV-Vis spectroscopy. Kinetics studies were carried out to establish the removal efficiencyand kinetics parameter for removal of 2,4-DNA. The batch adsorption studies of 2,4-DNA, showed that composite follows pseudo second order kinetic.The high surface area of nano-composite along with catalytic properties makes the composite material suitable for removal of explosive under ambient conditions.

Synthesis of new high energy molecules: Focus on one tetrazole derivative and generation of new structures

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Keywords: energetic material; tetrazole; imidoyl azide; insensitive material; artificial intelligence.

One of the major challenges in the chemistry of high energetic molecules is to find a substance with higher performances than current explosives. The latters, commonly used in civilian and military applications, are appreciated for their stability, ease of processing, and energetic features. However, with the development of new types of weapons and missiles, customers in the defense industry are looking for materials that surpass the current technologies by using original functional energetic molecules exhibiting increased key performance indicators. Also, by pushing the limits of modern weapons (speed of missiles, depth of submarines...), the new molecules should be more insensitive to external stresses than currently used explosives. In this work, the synthesis of the N,N′-bis((1H-tetrazol-5-yl)methyl)nitramide (BTMNA) suggested by Shreeve et al. in 2021 will be studied more carefully with a focus on the zinc-tetrazolate intermediate that has not been described previously in the literature. Sensitivity data and a suggested structure and mechanism for the intermediate will be provided as well as the challenges tackled during the scale-up of the synthesis. Another way to find new, insensitive and highly performant molecules is to use Artificial Intelligence (AI) not only to evaluate the energetic performances of molecules but also to generate innovative structures. Using databases and a set of performance and structural criteria, new molecules could be expected and the ultimate goal is to find a simple synthetic route for the most interesting ones.

Radiative and reactive coupling of lightning to electro-explosive devices in storage

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Keywords: electro-explosive devices; lightning protection; HERO; munition storage.

We theoretically study the absorption of radiative and reactive electromagnetic fields by electro-explosive devices (EEDs) in a munition storage struck by lightning. We find that reactive coupling in the near-field dominates for high resistance EEDs, while radiative coupling in the far-field from the strike location dominates for low resistance EEDs. Surprisingly, both couplings are substantially weaker than previously estimated. This is because the strike duration is long compared to typical electromagnetic response times. This lowers reactive absorption due to saturation of the electro-explosive device capacitance, while radiative absorption is low because the strike mostly emits low frequency modes with wavelengths longer than the dimensions of the munition storage.

Experimental analysis of liquid jet propulsion systems effects on IEDs casing materials

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Keywords: neutralization device; water jet; case material influence; IED.

One of the common methods for neutralizing Improvised Explosive Devices (IEDs) involves the use of projectile and liquid jet disruption. Liquid jet disruption can be achieved using disruptors or systems that harness explosion energy for propulsion, the latter being either omnidirectional or with directed action. The requirements for neutralizing IEDs refer to interrupt functions or separate components to prevent an unacceptable detonation. Although there are such neutralization systems, the literature is not very rich when it comes to aspects related to the velocities of the liquid jets and their action on casings and possible initiation of the IEDs. In these conditions, the paper presents the results of experimental research conducted by the authors on explosive propulsion systems of both omnidirectional and unidirectional types, with capacities of 0.5, 1, and 2 liters. The research aimed to establish the minimum distances at which the initiation of the detonator of the IEDs occurs under liquid jets and their ability to perforate casings of various thicknesses made of wood, metal, polycarbonate, and textile/leather materials. The obtained results showed that unidirectional explosive propulsion systems of liquid jets can be successfully used for the neutralization of IEDs.

A method for analysis of chiral molecules for the purpose of property prediction of EMs

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Keywords: ML; SMILES; chiral; density.

Nearly every molecular crystal structure solved by X-ray diffraction has been deposited in the Cambridge Structural Database (CSD). The CSD therefore enables large scale data analysis and machine learning (ML) based on real, isolated materials. This database is especially useful for energetic material research because each molecular structure includes crystal densities, one of the most important characteristics for understanding the performance of energetic materials. CSD allows for the export of large numbers of structures as simplified-molecular-input line-entry-system (SMILES) strings, but three-dimensional information such as chiral centers are generally lost during this translation. This work describes a method for the translation of CSD entries to stereospecific chiral strings that we anticipate will be useful for the development of better ML models of EM properties.

Composition for cooling of pyrotechnically generated hot aerosols

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Keywords: aerosol forming composite; cooling pellet composite; aerosol generator; aerosol; halon alternative.

Technology based on condensed aerosol has become increasingly popular as a Halon substitute for fire safety application in enclosed spaces. Aerosol forming composite (AFC), a pyrotechnic based component of condensed aerosol based fire extinguishing system (CAFES), burns to produce hot aerosols [1]. Aerosols that are produced must be cooled to prevent the possibility of secondary fires. The temperature of hot aerosol was recorded a maximum of 1200°C [2]. Therefore, cooling pellet composite (CPC) tablets must be positioned after AFC in order to absorb heat of hot aerosols. The integration of cooling pellet composite tablets into a CAFES system significantly enhances its heat management capabilities. The use of cooling tablets in CAFES systems is supported by several aspects, which contribute to enhanced thermal control. The cooling tablets possess the ability to reduce the temperature of a hot aerosol, either through the process of endothermic decomposition or by a phase change of ingredient of cooling composite.The cooling tablets also possess the capacity to decrease the concentration of harmful gases released during the combustion of aerosol-forming composites. MnCO3, basic MgCO3 based CPC were developed. By progressively incorporating magnesium carbonate, a range of compositions were generated, and their thermal properties were evaluated by means of TGA-DTA. At a MnCO3 to MgCO3 ratio of 35:50, the highest endothermic behavior was observed, with a ΔH value of 550 J/g. The binder ratio was also subsequently optimized. Using the UTM machine, the compressive strength of the tablets was determined. Compressive strength of 93 MPa was attained through the best combination of hot PVA and sodium silicate in the proportions of 4:2.Thermal clarance study was also performed to determine the best ratio of AFC:CPC. By employing these cooling tablets in CAFES of 0.1 kg AFC capacity, the temperature of the hot aerosol reduced from 1209 to 448°C.

Ballistic modifiers for nitrocellulose gunpowder

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Keywords: gun powder; modifiers.

The research deals with the synthesis and application of esters of diethylene glycol and nitrobenzoic acids. These compounds can be used in smokeless propellants as combustion modifiers that influence the burning character of the propellant. Diethylene glycol-bis(nitrobenzoates) have a higher energy content and a more favourable oxygen balance than currently used modifiers Centralites and Akardites. Diethylene glycol-bis(2-nitrobenzoate), diethylene glycol-bis(3-nitrobenzoate), diethylene glycol-bis(4-nitrobenzoate) and diethylene glycol-bis(3,5-dinitrobenzoate) were prepared by the reaction of nitrobenzoyl chlorides with diethylene glycol. The materials were applied to the surface of the grain of smokeless powder of the D090 type (single-based, nitroglycerine soak tube grain propellant) and tested in a weapon assembly for calibre .338 Lapua Magnum with a projectile weighing 19.44 g and a diameter of 8.6 mm. The shooting took place at temperatures of -54 řC, 21 řC and 52 řC. The results of the shooting show that diethylene glycol-bis(nitrobenzoates) have a lower (and therefore more advantageous) temperature coefficient than Akardite II. Diethylene glycol-bis(3-nitrobenzoate) gave the best results, with a temperature coefficient lower than other derivatives at 52 řC.

Dive into the thermal realms: Analyzing combustion and temperature characteristics in silicon-based compositions for time-delay detonators

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

This research delves into the combustion kinetics of silicon-based mixtures with bismuth(III) oxide (Bi2O3), antimony(III) oxide (Sb2O3) and lead(II,IV) oxide (Pb3O4), for the development of gasless time-delay detonators. The study aims to explore compositions that exhibit combustion rates independent of pressure inside the detonator. The combustion rates of the silicon mixtures were systematically studied, revealing distinct ranges for each composition. The Si/Sb2O3 mixture demonstrated combustion rates ranging from 8 to 35 mm/s, while Si/Bi2O3 exhibited rates of 15 to 110 mm/s. Notably, the Si/Pb3O4 composition showcased the highest combustion rates, ranging from 35 to 175 mm/s. The variations in combustion rates were attributed to the unique quantitative compositions and densities of each mixture. Additionally, temperature profiles for each composition were obtained using a thin thermocouple Pt-PtRh. These profiles offer valuable insights into the thermal dynamics of the combustion process, enhancing our understanding of the energetic properties of the silicon-based mixtures. Furthermore, the investigation involved measuring the heat of combustion across a broad range of quantitative compositions. The gasless combustion of each composition was verified through Differential Thermal Analysis (DTA) and X-ray Diffraction (XRD) techniques. The determination of qualitative combustion product compositions facilitated the calculation of adiabatic temperatures. To complement the quantitative findings, Scanning Electron Microscopy (SEM) images of the combustion products were obtained, providing visual insights into the morphological characteristics of the resulting structures. The use of silicon as a common fuel in these compositions contributes to the diversification of available pyrotechnic options for time-delay detonators. This study not only expands our understanding of combustion kinetics but also highlights the potential applicability of silicon-based mixtures in the field of energetic materials.

Study of explosion-generated plasma, it's velocity and effects upon collision

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Keywords: explosion-generated plasma; EGP; detonation; optical measurement.

Explosion-generated plasma is formed when the detonation wave exits condensed high explosive and compresses air surrounding the charge. It is a less known detonation phenomenon. It is naturally unstable, and it is reported to exist only for hundreds of nanoseconds. It however can be stabilized by leading the plasma through a tube attached to the charge. Interestingly, this leading tube doesnt̊ have to be made from a tough material, it can be thin plastic, glass or even a paper. This work is about measuring the velocity of created plasma in different geometries and studying the effects of its collision with a solid material. Velocities exceeding 10 km/s were measured and with varying geometries, different damage patterns on the witness plate were observed.

Tailoring the properties of ADN using co-crystallisation

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Keywords: ADN; ammonium dinitramide; co-crystal; energetic material; crystal engineering.

Co-crystallisation is a technique that can alter the performance properties of existing energetic materials (EMs) by changing the physical and chemical properties of crystalline solids. Ammonium dinitramide or ADN is a white salt comprising ammonium ions and dinitramide ions. ADN is a powerful oxidising agent because it has a high oxygen content. It also has high nitrogen content and is a green propellant because it is halogen-free. However, is very hygroscopic and has a relatively low melting point. In terms of sensitivity, ADN has a low impact sensitivity compared to ammonium perchlorate (AP). The drawbacks are the main problem of using ADN. In the past decade, there have been several reports about co-crystals of energetic materials, but interestingly there are only three concerning co-crystals of ADN. Moreover, three of them successfully used neutral molecules as the co-formers. In this research, the first co-crystals of ADN with other energetic salts have been successfully synthesised via crystal engineering. The crystals were studied by single-crystal X-ray diffraction. The physiochemical and energetic properties, including density, thermal stability, hygroscopicity, impact sensitivity and calculated energetic performance (e.g., detonation velocities and detonation pressures) of ADN could be adjusted using crystal engineering. The new components exhibit favourable physical and energetic properties, which are improved over ADN.

Synthesis and characterization of ^{13}C isotopically labeled $^{13}C_2$-FOX-7 (1,1-diamino-2,2-dinitroethylene)

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Keywords: energetic material; FOX-7, isotopic labeling; kinetic isotope effect; synthesis.

In order to investigate the kinetic isotope effect of 13C-labeled compounds on their properties, 13C-isotopically labeled 1,1-diamino-2,2-dinitroethylene (FOX-7) was synthesized and studied. Since the regular synthetic route to FOX-7 starts from 4,6-dihydroxyl-2-methyl-pyrimidine, which is not commercially available in labeled form, a different synthetic route had to be found. The synthesis was designed to start from 1,2-13C-labeled acetonitrile and lead to the known FOX-7 precursor 4,6-dihydroxyl-2-methyl-pyrimidine via a two-step process. The properties of the double 13C-labeled FOX-7 were investigated and compared with the deuterated and unlabeled version of the compound.

Amine oxidation under challenging conditions: Implementation of a flow-chemistry procedure for 3,4-dinitrofurazan synthesis

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Keywords: 3,4-dinitrofurazan; flow-chemistry; N-oxidation.

3,4-Dinitrofurazan (DNF) is both a liquid energetic material with unique properties and an excellent starting material for synthesis. Its batch synthesis is hazardous and time consuming. Therefore, we recently developed a novel microreactor based flow-chemistry procedure for the oxidation of DAF with commercially available hydrogen peroxide (70%) and concentrated sulfuric acid at elevated temperatures up to 60 řC. A yield of 32% DNF was received in preliminary experiments exploring suitable parameters for future studies. The herein presented process significantly increases safety in providing DNF on a laboratory scale and does not require the use of elemental fluorine or unusual reagents.

Experimental investigation on door breaching using explosives and its effects on room occupants

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Keywords: door breaching; explosive charge; water jet propulsion; metal door.

Among the methods for creating breaches in metal doors, the one using explosives is as rapid as it is demanding, both in placing explosive charges based on the door type and also regarding the effects on the intervention team and personnel behind the door. On the other hand, among the existing explosive charges, those propelling water jets and producing a pushing effect on the door are the most widely used, primarily due to their utilization of small amounts of explosives and minimal impact on the intervention personnel. Despite the numerous systems developed globally, the dependence on the door sheet type, the positioning of the explosive charge, and the effects on the intervention team and room occupants are aspects that require continuous research. This paper presents the results of experimental research regarding the creation of breaches in metal doors using explosive devices for water jet propulsion with an asymmetric closed sandwich configuration. The research is focused on metal doors, where the door face either is a continuous sheet of metal or comprised of parts made of Medium-Density Fiberboard (MDF). The explosive charges consist of a maximum of 25 g PETN in the form of a detonating cord and are placed in the locking system area. The effects of water jets on the neighboring door and occupants behind the door are monitored. Additionally, the effect of a delay on the order of milliseconds between charges is considered when two explosive devices are used. The obtained results show that although the explosive devices and their placement have the effect of creating the breach in the door, the effects on room occupants can be significant and must be taken into account when deciding to use such breaching methods.

Characterizing the shock sensitivity of HMX using laser-driven flyers

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Keywords: laser-driven flyer; PDV; shock wave; initiation.

Improving the safety of the shock initiation of energetic materials is an advantage brought by the use of laser-driven flyers. The implementation of this technique into a usable detonator requires a rigorous characterization of the energetic material's shock sensitivity. Using a Nd:YAG laser (1064 nm, 550 mJ, 6 ns pulse duration) in confined interaction to generate flyers with a diameter of 1 mm punched out of metallic coatings deposited onto 1 mm-thick H-K9L glass windows, go no-go tests were conducted on a HMX explosive charge. Flyer velocity was recorded using Photon Doppler Velocimetry (PDV) and critical initiation curves were obtained for different flyer thicknesses. Experimental results were compared to several energy criteria. Results showed better correspondence with Bowden's criterion. Better results were achieved for all criteria when excluding thicknesses where the flyer behaves as rod. Only one-dimensional and two-dimensional criteria were used in this work. Knowing that most laser-driven flyer exhibit some form of curvature, further studies will be necessary to determine the consequences of flyer curvature on shock initiation by laser-driven flyers.

Coagglomerated crystals of attractive nitramines in nitrocellulose gunpowder: A technological application

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Keywords: burn rate; co-agglomeration; co-crystal; gun powder; nitrocellulose.

Present study proven nitramines can qualitatively replace nitroglycerin in binary powders. Coagglomerated crystals (CACs) of RDX/BCHMX, inserted in this sense into gun powder, practically make double base powder type D063 charge and barrel length. During study, the samples also show that adding 10% RDX to the propellant does not increase the powder specific energy over the nitrocellulose one. The intra-ballistic model [1, 2]] of Kusák et al. compared theoretical projectile velocity and powder gas pressure to ballistic bomb (closed vessel) measurements and calculated characteristics are compared. Pressure consolidation reduces projectile velocity by 10 m.s-1, where pressure and burnt charge percentage are similar. Thus, adding this much RDX does not improve propellant performance. Instead, ECL gun powders with more RDX or combustion moderators may perform better. To correct the powder mass RDX deficiency, 2% BCHMX was added. This very small addition of BCHMX decreased values needs to be compensated by heavier weighting leads to less gun powder mass burned at the shot than in samples. Powder flashes forward after burning. In military ammunition, this is nearly unacceptable. Coagglomerated processed nitramines RDX/BCHMX performed better. The propellant's 7.62x39 cartridge assembly gave the best projectile velocity and powder gas pressure calculations. Here, BCHMX improves RDX powder mass combustion at 2%. As demonstrated powder is stable at various temperatures, ballistics would be extremely beneficial if ammunition temperature is a factor comparing 7.62x39 mm cartridge theories to bullet assemblies.

Toward estimating explosivity

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Keywords: explosivity; small-scale.

There is a need for small-scale (gram) tests that accurately predicts large-scale (kilogram) detonation performance of energetic materials. This is important to those involved in safety, performance, and even, regulations. Here we report small-scale (½", 1.27 cm diameter) detonation tests and the degree to which they reflect large-scale results. Of particular interest is ammonium nitrate and various formulations thereof.

Experimental characterization of emulsion explosives with inert additives

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Keywords: emulsion explosives; inert additives; detonation; characterization.

Emulsion explosives (EEs) are widely used in the industry, mostly due to their widespread applications, thus continuous progress has been made to characterize EEs and to maximize their potential. Although there is relevant information regarding the impact of energetic additives on high-density EEs, there is a dearth of information on the impact that non-energetic additives have on low-density EEs detonation process. In this work, it was performed an experimental characterization of the detonation velocity and pressure parameters of low-density EEs, using EPS as a non-energetic additive. The concentration of EPS in the EEs varied from 0% up to 4% and, consequently, the EEs density ranged from 1.12 g/cm3 and 0.49 g/cm3. Using a cylindrical charge, coupled with LEDAP standard multi-fibre optical probes, it was possible to achieve a quasi-continuous and simultaneous measurement of the EEs detonation velocities (2970 m/s up to 5580 m/s), and the velocity at which the shock wave propagates through an inert material, which allowed, by applying the impedance matching technique, the determination of the detonation pressure generated by the EEs (3.3 GPa up to 11.7 GPa).

A high-pressure structural study of potassium dinitramide

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Keywords: KDN; high pressures; phase transition; single-crystal X-ray crystallography.

This paper reports the effects of elevated pressures on the crystal structure of potassium dinitramide – an energetic material that is a precursor for ammonium dinitramide and which has been considered as an oxidiser in its own right. The smooth variation in unit-cell parameters provided no evidence for a phase transition up to 10.5 GPa. The variation in unit-cell volume was fitted to a 3rd order Birch-Murnaghan equation of state.

Towards a machine learning method to rationalise the impact sensitivities of energetic materials

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Keywords: impact sensitivity; machine learning; MLR; linear regression.

The experimental development of new energetic materials (EMs) is often hindered by strict safety and performance criteria. The results of tests for impact sensitivity (IS), among other safety measures, are greatly affected by variations in many sample properties and testing conditions, for example, temperature, sample purity and grain size. To mitigate these issues in the development of new materials, it has become important to be able to predict properties of EMs before manufacture, i.e., by computational modelling and screening. A predictive model for IS, which uses density functional theory and is based on the vibrational up-pumping method of energetic impact initiation, has been produced and tested on a wide range of EMs. Consequently, this model can be effectively used to predict if a material is a primary or a secondary energetic when the crystal structure of the material is known. Given that impact sensitivity is a material property, modelling using the solid-state crystal structure is the ideal standard for predicting impact sensitivity. However, a faster method which uses only the molecular structure could be more useful from the perspective of designing new materials. This work discusses a method of predicting a material's impact sensitivity using a multi-variate linear regression approach, with the aim of discovering the molecular properties which modify impact sensitivity.

Crystallization agents for ADN melting droplets

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Keywords: crystallization agents; melt emulsion.

Ammonium dinitramide (ADN) is a breakthrough green oxidizer in solid rocket propellants and a promising candidate for replacing environmentally harmful ammonium perchlorate, which is why current research is focusing on propellant formulations with ADN. Spherical ADN particles are required for embedding in the matrix of a solid propellant. Fast and controllable crystallization is therefore crucial for the quality of the so-called ADN prills. The effect of various additives was tested and categorized according to their effect. For this purpose, ADN droplets were examined both in the isolated ADN melt droplet and in the emulsion crystallization process.

Laser-driven flyer experiments: analogy with Gurney high explosive plate acceleration model

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Keywords: laser shock wave; PDV; high explosive; Gurney model.

The sustainability of satellites is threatened by the growing number of space debris in low-Earth orbit, which can collide and damage them. Understanding the mechanisms involved in such hypervelocity impacts (HVI) is essential to improving space shielding technologies. To experimentally investigate HVI, double-stage launchers can be used, propelling millimetric projectiles at very high velocities, reaching up to 8 to 10 km/s. Alternatively, high-power lasers may replicate similar characteristics of HVI, such as target craterization and debris cloud ejection, but with firing rates and equivalent speeds far superior to those of launchers. The laser sources can also be employed to launch small projectiles at very high speeds by an ablation process or to generate local severe pressure states useful in the determination of equations of state under shocks. This work aims to investigate the hypervelocity fragment ejection generated after a laser ablation. The conducted experiments employ the BELENOS facility at ENSTA Bretagne, France, having 1064 nm Nd: YAG pulsed laser generator with a full width at half maximum pulse duration of 7.5 ns ± 0.5 that can deliver a maximum energy of 3 J ± 0.05. The target is made of pure aluminum with two different thicknesses, respectively of 40 and 100 micrometers. Using a laser fluence from 10 to 50 J/cm2 with a 3.5 mm focal spot, the ejection reaches a velocity range of 1200 to 1600 m/s for the first sample, and a range of 400 to 800 m/s for the second one. The material velocity of the flyer's rear surface over time is captured by a Photonic Doppler Velocimeter (PDV) and is correlated with recordings from an ultra-high-speed camera. Fracture morphology of the specimen is then analyzed to identify specific patterns. Finally, since high explosives are also an alternative way to propel plates, an analogy is made with the Gurney's plate acceleration model.

A picture of the scientific explosives community before artificial intelligence takes over everything

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Keywords: explosive; scientific community; artificial intelligence.

If one thinks that artificial intelligence (AI) is the latest discovery, one may be in for a surprise. Application of AI in the field of explosives, understood as the use of neural network, is an idea over 30 years old. Just view a report from DTIC dated 1992, i.e. ADA250658. On the other hand, the beginning of the commercial use of neural networks goes back about 60 years. The key factor affecting the significant changes we observe today is AI achieving such a high level of development that this technology can be used everywhere and by everybody. Moreover, AI ceases to be a simple tool in human hands and becomes a human manager. Unfortunately, as was suggested last year at NTREM2023, each of the researchers had to face the problem of insufficient competency (too little knowledge and few co-workers) when confronted with the possibilities of AI. Examples of the above mentioned issues are presented in this work. The main issue addressed in this paper is to determine the potential of scientists, researchers and students dealing with explosives, to overcome contemporary challenges of conducting scientific work, no worse than that of AI. Most attention was paid to the surveys received from NTREM2023 participants and obtained through them from other researchers.

Evaluating the comparative potential of two indigenous microbial strains for degradation of 2,4,6- trinitrotoluene (TNT) and their biotransformation mechanisms

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Keywords: 2,4,6-trinitrotoluene; biodegradation; metabolites; high energetic material; microbes.

2,4,6-Trinitrotoluene (TNT) is a high energetic explosive compound with widespread military and civil applications. Its inadequate management and handling during manufacturing, transportation, exercising, demilitarization and detonation practices often lead to contamination of environmental matrices like soil and water. Environmental Protection Agency (EPA, 2014) has categorized TNT as a group C carcinogen, and a high toxic explosive which may lead to detrimental health effects, including anemia, cataracts, liver damages, and reproductive and immune system impairments. EPA has recommended a lifetime health advisory guidance level for TNT in drinking water as 2μg/L and set soil screening level of 19mg/Kg in residential and 79mg/Kg in industrial soil. Therefore, it is crucial to mitigate the negative impacts and possible associated risks to protect the environment. Microbial remediation can be an effective and sustainable option for clean-up of explosive contaminated sites as it promotes both environmental and economical aspects and has a lot of public acceptance. The current study was carried out with an objective to evaluate the potential of two indigenous microbial strains, Paenibacillus dendritiformis and Arthrobacter subterraneus which were isolated from an actual contaminated site for the degradation of TNT. The experimental studies involved assessing their ability to uptake the explosive as carbon and nitrogen source in controlled conditions in aqueous medium. A 30-days shake flask experiment was conducted under varying concentrations of TNT i.e. 60, 80, 100, and 120 mg/L. The reduction in concentration and biotransformation in secondary metabolites were obtained using high end instruments like High Performance Liquid Chromatography (HPLC) and Liquid Chromatography Mass Spectroscopy (LC-MS/MS). A degradation of 52 to 92% was achieved by Paenibacillus dendritiformis whereas, 52-65% was achieved by Arthrobacter subterraneus at different concentrations. Results confirmed the Paenibacillus sp. as better performer in degradation of TNT revealing its potential to remediate the explosive contaminated sites through microbial remediation technology.

Improving the precision of blast-induced seismic effect measurement results

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Keywords: blast-induced vibrations; peak particle velocity; charge weight per delay; atypical values.

Blasting is a commonly used technique in mining, construction, and geotechnical projects for breaking rock. While it is cost-effective, it can also have several negative impacts on the surrounding environment. These impacts include fly-rock, air blast, and blast-induced seismic effect, with the latter being the most significant. The seismic effect of blasting can cause ground vibrations that may lead to damage to nearby structures or affect the stability of the ground. However, not all measurement records are appropriate for calculations related to the seismic effect of blasting. A series of research and test blasts were carried out to assess the advantages of utilizing a larger number of instruments in a single measurement line. The focus was on determining the optimal positioning of these instruments and developing effective strategies for handling any outliers that might arise during the process. The results of these tests will enable us to refine our data collection methods and improve the accuracy of our measurements going forward.

Evaluating the effect of structural reorientation to thermochemical and energetic properties of 1,4-Diamino-3,6-dinitropyrazolo[4,3-c]pyrazole

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Keywords: LLM-119; fused rings; azole; structural isomers; detonation properties.

1,4-Diamino-3,6-dinitropyrazolo[4,3-c]pyrazole (LLM-119) and its structural isomer 3,6-dinitropyrazolo[3,4-c]pyrazole-1,4(6H)-diamine were designed by structural reorientation of the fused pyrazole rings and their respective substituents (-NO2 and -NH2). The structural reorientation involves structural rearrangement, which results in different structural isomers. Employing this approach, six structural isomers of LLM-119 were designed. The effect of structural reorientation (isomerisation and derivatives) on the enthalpy of formation, detonation properties, impact sensitivity, and density of these molecules is studied Computationally. The computational methods used in this work yielded results that are close to the literature values with a relative error of 2% for enthalpy of formation, 2% for density, 0.05% for detonation velocity, and 4% for detonation pressure. The correlation of the structural reorientation to the calculated thermochemical and detonation properties of the molecules indicated that molecules with a -NO2 group attached to a Carbon atom and -NH2 connected to a Nitrogen atom maximise the enthalpy of formation and detonation velocity. The joining of pyrazole molecules has less effect on these parameters. The data shows that density and detonation pressure improved when both -NO2 or -NH2 functional groups were on the same side of the molecular structure. The structural reorientation gave rise to 3,4-dinitropyrazolo[3,4-c]pyrazole-1,6-diamine which exhibited optimal density and detonation performance compared to other molecules.

Electrochemical synthesis of energetic materials and high-nitrogen compounds

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Keywords: electrochemical synthesis; thermally stable; high-nitrogen; energetic salts.

Herein, we have demonstrated the electrochemical synthesis of novel insensitive energetic materials in aqueous media at room temperature using non-toxic and environmentally friendly electrolyte. 3,4,5-triamino-1,2,4-triazole (guqnazine) was anodically oxidized to yield the azo-coupled energetic material 4,4‘,5,5‘-tetraamino-3,3‘-azo-bis-1,2,4-triazole (TAABT). TAABT was then used to produce a series of energetic salts. The sensitivities of TAABT and salts were characterized via DSC/TGA, BAM Impact, and BAM friction testing. All materials produced were analyzed via IR and multi-nuclear magnetic resonance (NMR) spectroscopy.

Investigation of the ability of nonel shock tubes to generate high pressure shock waves

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Keywords: nonel; shock tube; air shock wave; high pressures.

Generation of high pressures in the laboratory has been so far a non-trivial task to execute, as the usual way of the generation is either with explosives, or within a shock tube. Both options require rather specific infrastructure. In the case of explosives, a dedicated test range and with shock tubes high pressure certified equipment. To overcome possible local regulatory obstacles in setting up the latter, we propose to use Nonel as a safe, cost-effective and reliable source of energy for the blast wave generation. Nonel is a plastic tube filled with HMX/Al mixture, and its output consists of a shock wave and flame. The shock wave generated into a lab-scale shock tube with nonel could reach considerable overpressures starting at 25 kPa. Custom HMX/Al filled "nonels" were prepared to obtain higher overpressures, reaching up to 100 kPa. This concept advantageously uses nonel for generating shock waves in the shock tubes, thus avoiding necessity of bare explosives and detonators. Therefore, it provides a suitable way of shock wave examination in small-scale conditions, while preserving safety in terms of manipulation and sensitivity.

Excitation instead of heat and impact: A photocatalytic viewpoint on the laser ignition of energetic materials

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Keywords: laser ignition; photocatalysis; zinc oxide; pentaerythritol tetranitrate.

This work presents results demonstrating the efficiency of composite semiconductor nanomaterials for tuning the sensitivity of energetic materials to laser radiation. The synthesized nanostructures of zinc oxide doped with narrow-gap semiconductors or silver nanoparticles can act as a highly efficient PETN photosensitizer to laser radiation. The studied materials make PETN sensitive to both visible and infrared light, as well as, make it possible to use visible laser diodes with a power of about 10 W and IR industrial lasers with a power of about 1 kW as a reliable initiation instrument. Based on the obtained results, the general principles of application of semiconductor photocatalysts for laser initiation of energetic materials.

Influence of particle size on the thermal-mechanical properties of composite propellants

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Keywords: particle size; rubbery binder; HTPB; filler; glass transition temperature; bimodal.

Composite propellant consists of an energetic filler and polymeric binder which are intimately mixed, the interaction between the filler and binder affects the propellant rheology and mechanical properties, which are mainly influenced by the size of the particles and the packing fraction. This project aims to study the effect of the particle size on the thermal-mechanical properties of an inert model by mixing an HTPB binder with a filler of spherical glass beads using a resonant acoustic mixer, cast inside a square mold, and cured under vacuum. The main objective is to thoroughly study and analyze how different particle sizes influence the material's overall properties. By understanding these interactions, the aim is to optimize the formulation for potential applications in developing high-performance rocket motors. Four bimodal systems of coarse and fine glass beads were mixed for high solid loading. The density of the cured systems was studied by gas pycnometry, and it was observed that the density was slightly decreasing towards the top of the sample due to glass bead settling. The thermal properties were evaluated using differential scanning calorimetry, and the mechanical properties were assessed by dynamic mechanical analysis, the results suggested that glass transition temperature decreased as the particle size get finer, the storage modulus values increased with decreasing bead size in the systems, tan delta curves showed samples with larger particles have more damping characteristic.

The effect of graphene oxide (GO) on the bulk crystallization of ammonium nitrate

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Keywords: ammonium nitrate (AN); graphene oxide (GO); crystallization; phase transition; phase stabilization.

Ammonium nitrate (AN) is used extensively as a high nitrogen fertilizer and acts as an oxidiser in the energetic materials field. It is well known that its usage as part of a composite propellant is limited due to undesirable characteristics such as low burning rate, high hygroscopicity, low stability, and phase transformations. Even with these limitations, there is substantial interest nowadays in the development of AN based propellants as a replacement for Ammonium Perchlorate. This project studies the effect of Graphene Oxide (G/GO) on the polymorphic stability, phase transition behaviour and crystal structure of AN. G/GO exhibits a number of properties such as large surface area, energetic reactivity, good thermal conductivity and strong mechanical properties which may enhance the behaviour of AN. This study examines the crystallisation and behaviour of AN when doped with G/GO, using a range of crystallisation methods and considers the effect of growth conditions in addition to the role of G/GO as a nucleating agent. This work shows that the behaviour of AN when crystallised in the presence of G/GO differs from that where AN is crystallised onto G/GO surfaces.

Investigating the effects of natural aging on PBXN-111

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Keywords: polymer bonded explosives; aging; polymeric binder; antioxidant; plasticizer.

Polymer bonded explosives are commonly used in explosive ordnances owing to their high energy density and safety. However, their stability can be affected by external factors such as the conditions of the storage container and the surrounding environment. The study of the aging process of PBXs is therefore essential to accurately determine their stability and service life. This research investigates the chemical, thermal and mechanical degradation patterns of nine samples of PBXN-111 naturally aged between 3 and 20 years old. The findings of this study led to the conclusion that very little to no degradation was observed in PBXN-111.

Stability of the extruded double base (NC/DEGDN) modified with graphene oxide (GO)

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Keywords: ballistic modifier; stability analysis; activation energy; HPLC; nitrocellulose.

Double-base propellants (DBPs) have historically benefitted from including lead-based ballistic modifiers to enhance their combustion behavior. However, impending European legislation mandates the phasing out of lead in propellant formulations, necessitating the exploration of suitable alternatives. Graphene oxide (GO) has been introduced as a promising candidate, showing potential to improve the combustion performance of nitrocellulose microfilms. Before considering GO as a ballistic modifier for DBPs, it is crucial to examine the stability of such formulations thoroughly. This Work aims to elucidate the impact of GO on the fundamental characteristics and overall stability of DBPs. GO-based propellants were prepared, utilizing varying levels of oxidation (15% and 25-30% of O2). Artificial aging of the propellant at 80řC was conducted to provide valuable insights into their storage shelf life. Small-scale thermal stability analyses, including measurements of stabilizer content, activation energy for nitrate ester decomposition, and heat flow, were performed to assess the propellant's stability. Our findings indicate that adding GO to the propellant formulation does not compromise its stability. The activation energy analysis by differential scanning calorimetry revealed that the modified propellants exhibited stability similar to that of the unmodified formulation. The results from the stabilizer depletion assessment by liquid chromatography and thermal stability evaluation by heat flow calorimetry analyses confirm the propellant's ability to withstand storage for over a decade. This study contributes valuable insights to the use of GO as a valuable alternative lead-free ballistic modifier, highlighting its favorable impact on propellant stability and paving the way for future applications in the field of propulsion technology.

Assesment of a new solid thermobaric composition used for warheads loading

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Keywords: thermobaric composition; overpressure; piezoelectric transducers.

Thermobaric compositions are liquid and solid explosives characterized primarily by their shockwave effect. In this study, we propose the evaluation of a new solid thermobaric composition intended for use in warhead loadings. The primary advantages of solid thermobaric compositions lie in their ability to achieve a high loading density within ammunition and their minimal impact on the precision of strikes, unlike liquid compositions. The assessment of these new compositions is conducted through the analysis of overpressures over time, obtained under static conditions of an 'annular design' configuration, which was initiated by an electric cap. The variation in overpressure was recorded using piezoelectric transducers placed at different distances (2 m, 3 m, 3.5 m) and at the same level as the configuration. The recorded results have been used to assess the efficacy and destructive potential of thermobaric compositions present in warheads, a field that is constantly evolving.

Rheology study of HTPB prepolymer suspensions with different metal micro- and nano-sized particles

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Keywords: cast PBX and propellants; metal nanoparticles; HTPB; rheology; energetic performance.

The influence of the presence of metal powders, in the role of a fuel component, on the rheology of hydroxyl-terminated polybutadiene, HTPB, polymer binders for PBX explosives or composite propellants was studied. Different grades of micro- and nano-sized aluminum, magnesium or boron were used for the application in future optimization of existing cast formulations. Morphological analysis of Al, Mg and B micro- and nano-sized particles was done using scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS), for surface purity analyses of these metal particles. Rheological characterization of HTPB prepolymer suspensions, with and without Al, Mg and B particles, was performed using MCR 302 Anton Paar rheometer. Energetic performance of these HTPB/metal fuel mixtures was predicted using appropriate numerical models. The obtained results were analyzed for a prospective use of nanoparticle components in cast explosives or propellants.

Study of the RDX photolysis degradation products

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Keywords: photolysis; degradation products; RDX; FTIR.

The degree of contamination in areas affected with military activities is almost totally unknown. According to the future demands on the environmental policy and legislation it is of greatest obligation to conduct thorough research of aforementioned sites to determine the fate and environmental impact of energetic materials so that the remediation of soil and water could be achieved. This paper examines detected photolysis degradation products of RDX in prepared water sample using FTIR technique. The main goal of this study is to determine the influence of direct sunlight on the photolysis process of water samples prepared with RDX.

Recent developments on energetic di- and trisubstituted cubanes

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Keywords: energetic material; cubane; salt; DSC; NMR spectroscopy.

Although the cubane cage system was synthesized 60 years ago, some features are still unexplored. Apart from some carboxylates, no salts containing an anionic cubane moiety are reported. With the recent synthesis of cubane-1,4-dimethylnitrocarbamate (CMNC), several salts containing this energetic anion have now been synthesized and characterized. In addition, several tri-substituted energetic cubane derivatives were prepared. The compounds were characterized in detail, such as using heteronuclear NMR spectroscopy. Furthermore, the compounds were examined by DSC and sensitivity measurements for impact and friction.

Experimental research on TNT equivalent of different explosives based on air shock wave

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Keywords: detonation; air shock wave; TNT equivalent.

Equivalence is a convenient way to describe an effect, comparing it with an appropriate well-defined case. That approach is often used in the performance assessment of explosives. Since TNT is commonly used in explosive ordnance, other explosives are usually described using the TNT equivalent. It is especially useful in safety considerations for shock waves generated in air by an explosive, where simple calculation methods are developed for practical engineering usage. In this research, experimental overpressure and impulse of air shock wave for different explosive mixtures, including mixtures based on hydroxyl-terminated polybutadiene, HMX, ammonium perchlorate and metal powders, were compared with appropriate parameters and numerical models for TNT. The parameters of air shock wave were measured using piezoelectric sensors. The results were analysed using appropriate numerical methods in order to determine coefficients of TNT equivalence for considered explosives.

Assessing chemical inter-reactivity of high explosives. An outline for an adequate way

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Keywords: inter-reaction; reactivity; compatibility; reactivity limit values; weighting effects.

Assessing chemical stability and compatibility of energetic materials is already a long lasting task. At present, mostly traditional materials have been tested and evaluated. For them the established methods work mostly well, this also because of the already long and extensive experience with them. Newer materials as FOX-12, ADN, new organic oxidizers based on the nitro formate group, new energetics based on nitrogen-rich molecular groups as triazol and tetrazol are entering into the development and formulation departments and may reach or in part have reached demonstrator level and even in-service level. In part, some newer materials show good chemical stability, another part has to be evaluated with care. Both groups have in common that the experience with introduced and known material is not transferable directly. A more adapted assessment is necessary. Often the assessment is based only on methods like DSC and TGA, which provide results with small amounts of material in a short time, which is addressed as great advantage. With some evaluation software programs and some measurements a thorough evaluation and comparison is propagated. However, such fast determinations are by far not sufficient to get a correct information about thermo-chemical stability and compatibility.

This paper will clarify how assessments of thermo-chemical decomposition should be performed in order to obtain reasonable results. The often overseen effect of the temperature weighting caused by activation energy will be demonstrated and the consequences by this effect discussed. Next is the necessity to make the experimental determinations in such a way to reach enough conversion of the decomposition reaction. It is shown that the typical DSC measurements are not suitable to be used for sentencing the decomposition for lower temperature ranges at in-service conditions.

The next question is the about the limit values allowable with methods as gas generation, heat generation and mass loss. Until now, this question is not satisfactorily answered, especially with heat generation and gas generation, which are determined by heat flow microcalorimetry and vacuum stability test apparatus, respectively. A way to come to conclusive values will be outlined and discussed.

Exploring the mechanical characteristics of basebleed propellants: A comparative study

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Keywords: base bleed; propellant; ammonium perchlorate; mechanical properties; HTPB.

The present investigation scrutinizes the uniaxial tensile test characteristics of composite propellant formulations based on Hydroxyl-Terminated Polybutadiene/Ammonium Perchlorate (HTPB/AP), specifically designed for deployment in base bleed units for artillery projectiles. The base bleed unit functions by injecting low-velocity hot gas from the projectile's base, generated through the combustion of a low-burning rate composite propellant. This injection serves to eliminate the formation of a low-pressure zone and consequently reduces base drag, thereby facilitating an extension in range.

The study systematically explores the influence of varying ratios of additives, including cross-linker (Triethanolamine, TEA), chain extender (1,4-Butanediol, 1,4-BD), and bonding agent (TEPANOL), as well as diverse particle size distributions of Ammonium Perchlorate (AP), on the mechanical properties of the HTPB/AP-based propellant formulations. Through this investigation, the aim is to ascertain the relative changes in mechanical behavior to meet the requisite properties for the development of an efficient HTPB/AP-based composite propellant for base bleed units.

Identification and assessment of potential thermostable and powerful explosives

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Keywords: thermostable energetic materials; literature survey; database screening.

The quest for insensitive explosives has been running for decades. From the vast amount of research undertaken in this field, a number of valuable energetic compounds have evolved, which showed reduced sensitivity to various mechanical stimuli, such as impact and friction. However, the thermal sensitivity remains as one of the most difficult challenges to be taken, and known explosives exhibiting both a very high decomposition temperature (higher than 300řC) AND a high performance are very scarce. In order to identify new energetic compounds as realistic targets for demanding applications, two routes were explored: database screening and literature survey.

Development and characterization of novel polyurethane formulations for composite rocket propellants

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Keywords: polyurethane; composite rocket propellant; glass transition temperature; ballistic characterization.

Composite rocket propellants are heterogeneous energetic mixtures based on crystalline oxidizers, metallic powders, and a polymeric matrix. Nowadays, these composite formulations incorporate hydroxyl-terminated polybutadiene (HTPB) as polymeric binder, a class of butadiene-terminated oligomer, to provide optimal thermal and mechanical behavior. Novel polyurethane binder formulations comprising commercial polyols, an aliphatic isocyanate as a cross-linking agent, an organic catalyst and various plasticizers are reported here. The developed polyurethanes were investigated by specific analytical techniques: thermogravimetric analysis (TGA-DTG) and dynamic mechanical analysis (DMA). Furthermore, to demonstrate their applicability as binder for energetic composites, the optimal polyurethane formulation was employed in the development of novel composite mixtures that were further ballistically characterized.

Modeling and application of civil explosives in different types of soil

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Keywords: soil; explosive compaction; civil explosives; autodyn.

Civil or mining explosives have wide application in rock excavation and mining, but in the case of soils, their application is limited to some special blasting operations such as ground improvement. The three main applications of explosives in ground improvement are: soil compaction, mass excavation, and in situ pile creation. The suitability of explosives for each of these applications strongly depends upon the explosive properties and soil properties. The paper presents results of research of the soil compaction by civil explosives and modeling of that process using AUTODYN software. Explosive compaction has been performed in different type of soil. The calculated results from AUTODYN and the results obtained from in situ explosive compaction are compared and presented.

Influence of fillers on the mechanical and thermal characteristics of rocket motor liners based on HTPB

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Keywords: carbon black; hydroxyl-terminated polybutadiene; HTPB; nanoparticles; rocket motor liner.

Case bonded solid rocket motors hold significant importance in both the defense and aerospace industries which typically consist of an insulating layer, a solid propellant, and a liner layer serving as an adhesive between the insulator and solid propellant. The importance of liner layer is that it secures the propellant grain to the rocket motor chamber by adequate bonding. Therefore, determination of its properties is crucial for the design of a case bonded system. In this investigation, the aim was to assess the critical mechanical properties of five different HTPB based liner formulations under ambient conditions, as well as at elevated and reduced temperatures. The liners formulations incorporated micro carbon black, nano carbon black, nano silica, and nano titania as fillers. A comprehensive characterization study encompassing mechanical and thermal properties was conducted to evaluate the performance of these potential rocket motor liners. All mechanical properties of filled liner formulations enhanced significantly compared to unfilled formulation at all temperatures. At lower temperatures, mobility reduction of polymer chains as well as bond strengthening led to the enhancement in mechanical properties of all filled and unfilled liners. Contrary to that, at elevated temperatures, a decrease in the mechanical properties of all filled and unfilled liners has been observed due to the polymer chains being able to move more easily and the interactions at the molecular level being weaker. Augmentation in mechanical properties were more pronounced with carbon blacks as fillers. Thermal analyses of each formulation revealed that there are improvements in the thermal properties of filled liners compared to unfilled one. Three stage decomposition was observed for all liner formulations based on thermogravimetric analyses. Thermomechanical investigations revealed that thermal expansion of filled liners were lower than that of unfilled liner.

Risks in ammunition clean-up of the Black sea aquatoria

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Keywords: risk; ammunition; Black sea.

The paper discusses many years of experience in preparing and clean-up of ammunitions in the Black Sea aquatoria. A based sea level monitoring system was applied.The hydrography system used an echosounder with two frequencies 33 and 210 kHz, which provided information on the geometry of the sea bottom. The horizontal positioning control was carried out by a differential global positioning system (DGPS). The reference station type Trimble 4000MSK DGPS Reference Station was used. The system was based on the reception of GPS signal from satellites. The maximum number of satellites broadcasting GPS signals was between 24 and 30.

Influence of erosion-induced geometry changes on the flow vented vessel experiments

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Keywords: erosion; CFD; propellant; vented vessel experiment.

In the development of new, more powerful propellant charges the erosion of the gun barrel must be considered. During the combustion process high pressure is produced and hot gases cause erosive material removal within the barrel. Vented vessel tests are regularly performed to evaluate the erosivity of gun propellants. In these tests, a gun propellant is burned and the resulting combustion gases flow out of the combustion chamber through a metal nozzle. While giving a relative measure for the erosivitiy of gun propellants the transferability of the results to the conditions in a real gun and the dominant erosion mechanisms are still under investigation. The gas flow causes material removal of the nozzle, which is measured by weighing and is used to evaluate the erosion. In this work computed tomography (CT) scans are utilized to further quantify the erosion during the experiment. The removal of the material alters the geometry of the nozzle drastically, hence the flow conditions during the test change as well. This phenomenon has not been sufficiently investigated. The aim of this work is to investigate the influence of the geometry change on the resulting flow during vented vessel tests to better understand the mechanisms that lead to erosion. For this the CT scans were transferred to a 2D CFD grid and numerical fluid dynamic simulations are performed within the OpenFOAM framework.

LOVA propellants based on RDX and GAP energetic plasticizers

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Keywords: gun propellants; RDX; GAP; composite.

In this study RDX (cyclotrimethylene trinitramine) as an energetic filler and CA (cellulose acetate) plasticized with GAP (glycidyl azide polymer) as binder matrix were evaluated for low vulnerability ammunition (LOVA) gun propellants. A novel technique of precipitation was developed for the formation of micronic RDX crystals and simultaneous incorporation into the polymeric matrix. Initial ballistic investigations using close vessel firings were also performed, in order to comparatively evaluate the ballistic parameters of the new propellant.

A theoretical exploration of hexazine anion $[N_6]^{4-}$

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Keywords: hexazine anion; geometric characteristics; bonding nature; aromaticity; wavefunction analysis.

The unique ring structure of hexazine anion [N6]4− brings a variety of unusual characteristics and properties, which are quite worth to be explored. In this work, we present an extremely comprehensive and detailed investigation on almost all aspects of the hexazine anion, including geometric characteristics, bonding nature and aromaticity. We believe that our characterization of the hexazine anion will deepen researchers' understanding of this system, and thereby help them to utilize it in practice and design its various valuable derivatives.

A comparison of the acoustic performance of flash compositions used in firecrackers

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Keywords: report generation; firecracker performance; flash powder; air blast wave.

This study investigates the acoustic performance of flash compositions used in firecrackers, focusing on comparison of powdered metal fuel-based and organic fuel-based formulations. The research aims to characterize air blast wave parameters generated by explosions and compare the performance of different compositions. The performance of the flash powders was measured in prefabricated firecracker paper tube set up. Air blast wave parameters were recorded using a Piezotronics pressure sensor connected to a Dewesoft Sirius HS data acquisition device. The results indicate that metal fuel compositions, achieved significantly higher overpressures and impulses compared to organic fuel-based compositions. The latter exhibited about half the overpressures and one-third the impulses. While the organic fuel-based compositions may not be suitable for high-performance applications, they show potential for use in mid-range firecrackers. This work contributes valuable data on the acoustic characteristics of flash compositions, offering insights into their practical applications in pyrotechnics.

OPTIMEX: Detonation pressure measurement using stacked PTFE sheets

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Keywords: detonation pressure; shock velocity; nitromethane; fiber optic.

One of the methods for detonation pressure determination is based on the measurement of shock velocity in an inert material attached to the front surface of a cylindrical explosive charge. In this work, a stack of polytetrafluorethylene (PTFE) sheets was used as the inert material that produced light flashes on shock passage through each gap between sheets. The light signals were recorded by an axially placed plastic optical fiber and the OPTIMEX-8 passive light acquisition system. Limitations and reproducibility of this technique were investigated by testing nitromethane, a well characterized explosive, in explosive charges of 5 and 8 mm diameter with length to diameter ratio from 1 to 6. The measured results were validated by comparison with reference data previously obtained using impedance window and flyer plate tests.

Dynamic calibration and implementation of PVDF gauges for shockwave measurements

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Keywords: PVDF pressure gauge; shock tube; shock wave; measurements.

Measurement of shock waves characteristics like overpressure or impulse require specifics pressure sensors and acquisition devices. Piezoceramics sensors are commonely used in this way. Nevertheless, there cost and intriseque conditionning integration may not suitable with near fields applications. Piezoelectrics polymers like PVDF pressure gauges may be an alternative due to there cheep cost and manufacturing process but they need to be precisely conditionned (electrically and mechanically). In this context, we propose a methodology to calibrate these PVDF pressure sensors. The first part of the study presents various steps to build the PVDF pressure sensor, the conditonning electrical circuit, the insulation process and the mechanical integration. Then, we performed experiments on the shocktube facility at ENSTA Bretagne. This facility can generates two types of pressure sollicitations, relative to the length of the driver section : The shock configuration, with a pressure plateau, and a more realistic configuration, the blast (or Friedlander like) configuration. The intensity of the overpressure is ruled by the thickness of mylar sheets placed between the driver section and the test section. Six piezoelectrics sensors (PCB piezoelectronics) along the test section measure the incident pressure and one at the back, measuring the reflected wave. The uniformity of the shockwave is observed with shadowgraph technique recorded on a high-speed camera. All these informations coupled with analytical model of shocktube characteristics ensure the validity of the set-up. Finally, the signal of the reflected sensor is compared with the PVDF sensor signal. The analysis of the signals exhibit the dynamic response of the PVDF sensor, the characterization of the electrical noise due to the prior conditionning and the suitability of the methodology to measure reflected blastwaves

Experimental evaluation of detonation parameters in a single test

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Keywords: detonation; PBX; multi-fiber optical probe; meso-scale characterization.

Experimental determination of detonation phenomena is essentially focused on the measurement of detonation velocity, detonation pressure, detonation front curvature and Gurney energy. Many experimental methods based on electrical, optical, X-ray or magnetic phenomena have been developed, however, some of them need expensive equipment. One non-intrusive and precise method is based on an optical method associated with an electronic streak camera (ESC). This work presents the application of the multi-fiber optical probe (MFOP), which consists of a high spatial and temporal resolution optical method based on an optical fibers ribbon connected to an ESC for the characterization of the detonation process of a small PBX charge. The MFOP is based on 64 optical fibers having a diameter of 250 micro m, and is connected to an ESC without any intermediate optics and allows to record radiation phenomena emitting in the range of 360 - 700 nm. This method was applied to the simultaneous measurement of detonation velocity, detonation pressure field and detonation front curvature in PBX explosive charges. One part of the MFOP is fixed on the charge side to measure the quasi-continuous detonation velocity with a spatial resolution of 250 micro m, and the second part is fixed at the charge's end to acquire the breakout light, recording the detonation front curvature. When a set of polyimide layers (125 micro m of thickness) is mounted between the charge's end and the top of optical fibers, it allows the evaluation of a pressure field induced in the polyimide barrier by the detonation front. The present experimental method allows the meso-scale probing of the 3D reaction zone structure.

Dynamic vapor sorption study of MTX-1 alkali metal salt hydrates

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Keywords: DVS; MTX-1; hydrate; alkali metal salt.

The formation of hydrates is a common phenomenon in crystalline materials. The presence of crystal water greatly impacts the properties of the resulting materials, which in the case of energetic materials leads to a decrease in sensitivity, density, and performance. The formation of MTX-1 alkali salt hydrates, a category of poorly described salts of the perspective primary explosive, was studied by the dynamic vapor sorption method, which allows for a rapid investigation of water sorption and/or desorption of substances in small sample quantities and over a wide range of humidity. The compounds were also used as materials for the assessment of the method's practicality in the study of energetic materials hydrate formation. The alkali salts were characterized by DTA, FT-IR, and elemental analysis. The water content in the dehydrated salts was determined by Karl-Fisher titration.

Study of the gun powders ignition by laser beam in closed vessels

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Keywords: laser ignition; closed vessel; primer.

Last decades development in the field of lasers makes such devices more accessible and new applications can be imagined. The present study addresses the possibility of replacing the electric ignition of gun powders in closed vessel with the laser ignition. Both, powder direct ignition and indirect ignition based on an additional charge (the primer) were analyzed.

Towards finding lead-free ballistic modifiers in double-base propellants using computational modelling

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Keywords: ballistic modifiers; double-base propellants; DBPs.

Lead-based ballistic modifiers have been the industry standard for double-base propellants (DBPs) since the 1960s. They are known to modify the burn-rate in three distinct ways (super, plateau and mesa-rate burning), which together offers greater control of ballistic performance. However, the continued reliance on lead-based ballistic modifiers is problematic due to the inherent high toxicity of lead, and incoming REACH and UK REACH legislation will restrict their use. In efforts to find suitable alternatives, a computational model has been developed which accounts for the success of lead oxide as a ballistic modifier and allows for other metal oxides to be tested. It models the ballistic modifier in the presence of carbon and small molecules produced at the burning surface of the DBP during combustion. Following a study of selected metal oxides, this work looks at streamlining the computational method and further investigating additional metal oxides with the aim of understanding how they might impact the burn rate of DBPs.

Innovative coagglomeration method for producing the energy-safety balanced cocrystals of attractive nitramines

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Keywords: co-agglomeration; co-crystal; detonation parameters; impact sensitivity; nitramines.

The novel crystal engineering technique involves the co-agglomeration of energetic materials with co-precipitated micro-particles of nitramines, such as CL20, HMX, BCHMX, and RDX, using the slurry method to alter the energetic properties of these compounds. Here we discussed the fascinating structural changes and intriguing properties of freshly made co-agglomerated crystals (CACs). Crystal morphologies and packing can vary greatly, leading to differences in important properties such as density, melting point, impact sensitivity, and detonation characteristics. All the CACs exhibited co-crystal characteristics. Beyond these considerations, co-agglomeration offers a great chance to modify the essential characteristics and functionality of current energetic materials, and it is adoptable to scale up, along with the tremendous improvements over conventional crystallization. These preliminary results also imply that chemical engineering factors are involved in the preparation of CACs. It is possible to use this method for industrial-scale production with some technical optimization.

The influence of magnesium liner on artillery shell explosive disposal

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Keywords: numerical simulation; LS-Dyna; EOD.

In this paper, a numerical simulation model for impact between a magnesium liner and a steel plate was made, in order to study the effect of an ordinance disposal device on an artillery shell. The simulation was made using LS-Dyna software and aim to validate calculations and hypotheses regarding disposal of artillery shells using an explosive device. Geometrical model build in numerical simulation is composed from a cylindrical explosive device and a 9 mm steel plate, which represents the shell body of a medium calibre projectile. Thus, the obtained results shows that although it may represent a laborious study, it serves as a starting point for further research on unexploded ordnance disposal field, a current topic in today's world.

Energetic salts based on 5-(5-Amino-1H-1,2,4-triazole-3-yl)-1H-tetrazole with good thermal stability

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Keywords: energetic material; heat-resistant; nitrogen rich heterocyclic; zwitterionic.

Heat-resistant explosives play an irreplaceable role in special applications. Firstly, energetic salts with high thermal stability and energy performance, namely N2H5-ATT and NO3-ATT, were synthesized based on the amphoteric properties of 5-(5-Amino-1H-1,2,4-triazole-3-yl)-1H-tetrazole (H2ATT). And it was characterized through chemical (IR spectroscopy and single crystal XRD) and physicochemical analysis (friction, impact, electrostatic, and DSC testing). Research has found that it has high thermal stability, high heat of formation, and appropriate sensitivity. Their detonation performance (detonation velocity, detonation pressure, etc.) is calculated using the EXPLO5 program. Meanwhile, its detonation performance is comparable to high-energy potassium salts such as HNS, making it a promising heat-resistant explosive.

Synthesis and energetic characterization of borane-amines on high-nitrogen heterocycles

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Keywords: borane-amines; hypergols; high nitrogen content heterocycles.

Over the last several decades, borane-amines have gathered attention in a variety of fields ranging from hydrogen storage materials to hypergolic fuels. Current approaches to hypergolic fuels center about hydrazine systems, which are exceptionally toxic in nature. Borane-amines have advantages over hydrazine fuels, as borane-amines are generally markedly less toxic than hydrazine in addition to retaining hypergolic functionality. In this work, new borane-amines were synthesized on high nitrogen content heterocycles by reacting the parent amine with two equivalents of borane dimethylsulfide (BMS) in anhydrous THF. Isolation of the relevant borane-amine is achieved by diluting the reaction with hexanes, which precipitates out the requisite borane-amine. Chemical identity of products was confirmed by x-ray crystallography, TGA, HRMS, 1H NMR, 13C NMR, and 11B NMR, while energetic impact and friction sensitivity testing were used to identify sensitivity to physical stimuli. Most isolated borane-amines decomposed in the presence of atmospheric moisture, save one. Additionally, some became sensitive to impact and friction stimuli. However, all novel borane-amines identified in this work retain the characteristic hypergolicity with white fuming nitric acid (WFNA) which is expected for borane-amines.

Synthesis, thermal and spectroscopical properties of the cocrystal CL-20-MDNT

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Keywords: energetic material; crystal structure; cocrystal; CL-20; MDNT.

Comparing different solvents applied in cooling and evaporation crystallization methods, ethyl acetate was found to be a suitable solvent for the crystallization of the cocrystal of Hexanitroisowurtzitan (C6H6N12O12)-Methyldinitrotriazol (C3H3N5O4) in the ratio 1:1. The cocrystal is a promising candidate for an explosive material with a detonation performance superior to Octogen and improved sensitivities compared to pure CL-20. A phase pure product was obtained with a density of 1.86 g/cmş at ambient temperature. Raman spectra show a split of the signals attributed to the MDNT methyl group as well as shifts of 4-10 cm-1 for nitro group signals comparing pure MDNT with the cocrystal. Single crystal diffraction experiments confirmed space group P212121 for the crystal structure and offered input for further theoretical considerations. DSC measurements show a decomposition peak at 246 řC and a small endothermic signal at about 168 řC, linked with an irreversible phase transition and a reduction in volume, which is subject of investigations via in-situ diffraction and thermal analytic methods.

Innovative perspective on measuring the sensitivity of boron potassium nitrate to different stimuli

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Keywords: boron potassium nitrate; pyrotechnic; energetic material; sensitivity distribution function; FEST method.

Boron potassium nitrate is a pyrotechnic mixture often used as an ignition charge for rocket propellant igniters. Regarding energetic materials, safety is a limiting feature for use and is generally referred to in the form of sensitivity. Boron potassium nitrate is reported to be safe for impact, friction, and electrostatic discharge, according to the most commonly used methods. The first two parameters are well described in the literature, while the latter is not sufficiently detailed. For this reason, it was proposed to analyze the sensitivity to electrostatic discharge of a boron potassium nitrate composition and evaluate safety from an innovative perspective, using the FEST method. This method is efficient for its ability to create, with a low number of trials, a distribution function for sensitivity that considers the entire range of experiments but also guarantees confidence for the maximum likelihood estimation in the area of interest due to its procedure that focuses on ignition data overlap. The ESD results were presented as sensitivity distribution functions and suggest that the composition may not be as safe as usually reported.

60 mm thermobaric mortar round fragmentation effect

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Keywords: fragmentation; thermobaric.

One of the basic requirements for high explosive fragmentation projectiles is their fragmentation effect. The subject of the fragment formation process, known as fragmentation, and its optimization is an actual topic and has long been of interest in the military field. There are three categories of metallic casing fragmentation: natural, controlled, and preformed fragmentation. Due to the increasing number of conflicts in urban or built-up areas, the development of projectiles with controlled and preformed fragmentation with a defined lethal zone and a high density of effective fragments in this zone has been intensified in recent years. This paper is focused on experimental analysis of the 60 mm thermobaric mortar round fragmentation effect including fragment velocity measurement and verification of the lethal effect of individual fragments at four different distances from the point of mortar round detonation. Three different types of mortar shell casing designs were tested: shear-controlled grids on the outer surface of the casing, uniform thickness-controlled grid layer placed between the casing and explosive, and finally, an inner layer made of bearing balls in a polymer matrix inside the casing of the mortar round.

High stability N-rich energetic materials based on 5,5'-(1H-pyrazole-3,5-diyl)bis(4H-1,2,4-triazole-3,4-diamine)

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Keywords: energetic material; triazole; pyrazol; N-rich; crystal structure.

Improving the thermostabilities and the mechanical sensitivities to develop the heat resistant and insensitive N-rich energetic materials has become a new trend during recent years. Here, a novel N-rich energetic material, 5,5'-(1H-pyrazole-3,5-diyl)bis(4H-1,2,4-triazole-3,4-diamine) (N%: 64.10), was prepared through the introduction of an energetic pyrazol bridge to connect two diamino triazole groups, based on it, a series of energetic salts were synthesized and characterized. Additionally, the perchlorate salt, 4,5-diamino-3-(3-(4,5-diamino-4H-1,2,4-triazol-3-yl)-1H-pyrazol-5-yl)-4H-1,2,4-triazol-1-ium perchlorate, was investigated using the single crystal XRD to detailly figure out the internal molecular structures, also, the existence of huge hydrogen bonds shown in the crystal structure demonstrated it a heat resistant and insensitive energetic material. Interestingly, although 5,5'-(1H-pyrazole-3,5-diyl)bis(4H-1,2,4-triazole-3,4-diamine) exhibited a symmetrical structure, it cannot form a bivalent ionic salt, all derivatives manifested as monoionic salts. All the novel energetic materials in this study exhibited improved performances: superior heat of formation (908.8 1415.4 KJ mol^{-1}) to generate excellent detonation performances (Dv: 7850 to 8355 m s^{-1}, P: 21.46 to 25.55 GPa) with low mechanical sensitivities (IS > 40 J, FS > 360 N) and high decomposition temperatures (241 344 řC). Besides, non-covalent interactions were evaluated and discussed to explain the outstanding stabilities. The comprehensive performances of 5,5'-(1H-pyrazole-3,5-diyl)bis(4H-1,2,4-triazole-3,4-diamine) made it a promising high-stability energetic material.

Keyword Index

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