Abstracts of the 24th Seminar on

New Trends in Research of Energetic Materials

NTREM

Pardubice, April 6–8, 2022

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

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New Trends in Research of Energetic Materials

Held at the University of Pardubice

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

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Preface

The tradition of our annual NTREM seminars was disrupted two years ago by the Covid pandemic, which forced us to cancel the meeting in later stages of preparation in 2020 and to drop the idea of organizing it completely in 2021. With the pandemic slowly losing its strength the situation started to look quite promising and hence the preparation of the 24th seminar (it was originally supposed to be the 25th one) started in fall of 2021.

During the preparations, we were very unpleasantly surprised by Russia's unexpected attack on Ukraine, which made it impossible for Russian scientists to participate. We can only hope that the situation will calm down in due course and that our NTREM seminars will fully return to their traditional mission of bringing together young scientists and engineers from around the world.

This year's meeting is taking place in the worst conditions in the modern history of the Czech Republic and in one of the worst periods in Europe. This fact must not affect the creation of a traditionally pleasant meeting where young professionals from different countries will have the opportunity to meet and gain personal contacts that will develop into further cooperation.

One of the decisive factors enabling realisation of these seminars has been the financial assistance of well-wishers of this activity. The Seminar is sponsored by the following:

- Austin Detonator, Czech Republic;
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The efficient help in ensuring smooth and successful course of the meeting obtained from all these institutions is gratefully acknowledged. We greatly appreciate the continuing support especially after the two-year break. Thanks to this sponsoring we are able to keep the seminar easily accessible to young generation of students and researchers.

And traditionally, let mi thank the members of the Scientific Committee, the Organizing Committee, the authors of all the seminar papers and, last but not least, you, the participants of this seminar, for its success. I wish you big successes in your life and scientific work, a good health and goodbye till next April here at our University.

Pardubice, February 28th, 2022

Svatopluk Zeman

Structure-property relationships for multi-component crystals of nitropyrazoles

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Keywords: energetic materials; impact sensitivity; structure-property relationship.

Nitropyrazole group energetic compounds are promising candidates to replace conventional explosives, as they generally have positive heats of formation, good thermal stabilities, low friction and impact sensitivities, and high energetic performance. Co-crystallisation and salt formation offer a tuneable approach to enhance crystalline material properties. It has found ready application in the pharmaceutical industry, for instance, as a means to improve the solubility and processing of drug molecules. Recently, it became a useful tool for tailoring the properties of energetic materials.

Highly nitrated pyrazoles are expected to be high explosives and can be used as an ingredient of propellants. In this study, co-crystallisation/salt formation technique was applied on nitropyrazole based materials for improving a group of structure-property relationships. For this aim, 3,5-dinitropyrazole (DNP) and 3,4,5-trinitropyrazole (TNP) being a high energetic materials were combined with different pyridine derivatives. Totally, 4 novel multicomponent energetic materials were produced and investigated. Crystal structures, experimental impact sensitivities, thermal behaviours and energetic properties of these novel energetic materials were reported. Intermolecular interactions formed in these structures including hydrogen an halogen bonds were analysed. Structure-impact sensitivity relationships were explained using crystal structure properties including non-covalent interactions, crystal densities and packing motifs. Sensitivity of the novel structures were predicted with computational methods based on multiphonon up-pumping theory and experimental impact sensitivity results were correlated with calculations successfully.

Energetic functionalization of 2,5-diaminotetrazole

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Keywords: tetrazole; functionalization; X-ray diffraction; amination.

Tetrazoles are an unique class of endothermic compounds which can be used in all classes of energetic materials as a) explosives, b) propellants as wess as c) pyrotechnics. 1,5-Diaminotetrazole is a well known nitrogen-rich tetrazole compound which has been utilized for numerous derivatizations e.g. nitration, oxidation, salt formation or complexation. It is synthesized by different routes which all have some drawbacks a) oxidation of semicarbazide, b) amination of 5-aminotetrazolate, c) reaction of hydrazine with cyanogen bromide and d) diazotization of diaminoguanidine. For the first time we now were able to collect a large amount of its 2,5-diamionotetrazole isomere. Despite the long history of its synthesis, almost nothing is known about 2,5-diaminotetrazole and its derivatives. In this study, 2,5-diaminotetrazole is characterized in terms of its chemical and energetic points of view. Several energetic salts based on the 2,5-diaminotetrazolium, 2,5-diamino-4-methyltetrazolium and 1,3,5-triaminotetrazolium cations and respective energetic anions are investigated. All compounds were intensively studied through multinuclear NMR and IR spectroscopy, X-ray diffracion experiments, thermal stability testing using DTA and sensitivity measurements according to BAM standards. The detonation performances were calculated using the EXPLO5 code.

Effect of mechanical impact on PBX disk investigated by DMA

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Keywords: HMX-based PBX; mechanical impact; DMA; glass-to-rubber transition; modified Arrhenius.

One safety aspect during use of plastic bonded high explosives (PBX) is their resilience against mechanical impacts as they may happen by set-back of the HE charge during firing. To investigate this feature PBX disks with 140 mm in diameter and 5 mm thick where manufactured and, held in a fixture, exposed to projectile impacts to simulate the set-back effect The PBX disk was covered with a thin steel plate to simulate to some extend the base casing. The frame composition of the PBX is HTPB (hydroxyl terminated polybutadiene) based binder cured with IPDI (isophorone diisocyanate), HMX, plasticizer DOA (dioctyl adipate) and a phenolic antioxidant. The projectile impact was performed with such a velocity that the steel plate was not perforated but clear destruction effects on the PBX plate were created. The plate was then sectioned into DMA sample stripes with different distances to the impact center (DTIC). The DMA (dynamic mechanical analysis) measurements were done in torsion and the rectangular samples were about 10 mm wide, and 18 to 40 mm long. The temperature dependence was evaluated with a step-wise increase by 1řC from -120řC to +90řC. The deformation frequencies were in the range of 0.1 Hz to 30Hz with 9 frequencies in total and applied on each temperature step after an equilibration period. The measurements revealed a clear indication of changes with the DTIC. Observed was a shift of the glass-to-rubber transition temperature (GTR-T) to lower temperatures with decreasing DTIC. With each measurement frequency, a clear dependence of the GTR-T with DICT was found. The dependencies of GTR-T on deformation frequency are evaluated with two equations of type standard Arrhenius (providing f_0, Ea_f) and of modified Arrhenius (providing f_0M, Ea_0M and T_0M). The change of the parameters Ea_f and Ea_0M, T_0M are discussed in terms of DTIC.

Development of capacitive sensors for the study of detonation

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Keywords: capacitive sensor; detonation; detonation zone.

A novel capacitive sensor has been designed and manufactured to allow for spatially and temporally resolved measurements to be made of materials in the time before steady state detonation has developed. The sensors are driven by a high frequency waveform generator and then the effects of the conductive zone within the reaction front alter the shape of the waveform which is then detected using a high bandwidth oscilloscope. Details are given of the analysis routine, along with some examples of the results that are obtainable.

In silico mutagenicity prediction by similarity search and machine learning algorithm: Optimisation and validation of the method for High Energetic Materials

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Keywords: prediction; toxicity; mutagenicity; machine learning; HEM.

The European regulation REACh (Registration, Evaluation, Authorization, and restriction of Chemicals) has placed responsibility on industry to manage the risk from chemicals since 2006. In order to ensure a high level of protection of human health and environment, toxicity prediction methods are now a widely used tool for regulatory decision making and selection of leads in new substances design. These in silico methods are an alternative to traditional in vitro and in vivo testing methods, which are laborious, time-consuming, highly expensive, and even involve animal welfare issues. Many computational methods have been employed to predict the toxicity profile of substance, but they are mostly adapted to pharmaceutical molecules and not to High Energetic Materials (HEM).

In line with these restrictions, ArianeGroup set up a collaborative project with the French CNRS to develop optimized tools for the prediction of HEM properties, such as toxicity. Several in silico methods can be used to predict the properties of molecules, such as QSAR, Local QSAR, or Machine Learning. We already demonstrated that using Local QSAR allows for better predictions and a good reliability1.

We therefore developed a toxicity prediction tool based on the structural similarity search coupled with a supervised machine learning algorithm. The aim of this paper is to evaluate the performance of our method using learning curves and test databases. This evaluation showed a strong overfitting for the Ames test. An optimisation was therefore necessary to reduce the overfitting, which caused a decline in the generalisation capacity of the predictive model. The dimensionality reduction of the training set and the hyperparameters optimisation of the different algorithms showed a performance acceleration and a significant reduction of the overfitting. The performance of the predictive model was evaluated on a test set of HEM and compared to the results of other prediction softwares.

Quantitative properties through semantic learning

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Keywords: machine learning; natural language processing; energetics; impact sensitivity; detonation velocity; detonation pressure.

Material properties have almost exclusively been studied via natural science-based theoretical and experimental approaches. However, applying Natural Language Processing (NLP) tools to aid in the characterization, design, and discovery of energetic materials poses fertile new ground for research where linguistics plays a role. This paper will test if statistical relationships exist between the language used to discuss energetic materials and their fundamental physicochemical properties. First, we create a word space comprised of a corpus of over 10,000 open literature documents consisting of full-length journal articles, conference papers, technical reports, and patents. The corpus was developed following a standard text preprocessing pipeline. Word embedding models (word2vec and Glove) were then used to generate n-dimensional word vectors, which are mathematical representations of the words, in an attempt to capture the semantic content in the text. In parallel, we created a chemical space based on the chemical and physical properties of energetic compounds. The statistical nature of the chemical space arises from the variability of measured values of properties and the variability due to differences in the chemical composition of the materials. Statistical models were developed for both spaces separately and compared using Jensen-Shannon, Hellinger, and Wasserstein distances.

Performance properties for impact sensitivity (h_50), detonation velocity (D), and detonation pressure (P) were studied. Statistical comparisons between the word space and the chemical space distributions were performed using limited sets of reference energetics: 5 for h_50 and 15 for D and P. A surprising and remarkable degree of statistical equivalence was found, in some cases showing >90% confidence levels. This work posits a new means for using automated machine-assisted approaches to learn from technical documents and facilitate the search and discovery of new materials by discovering these statistical relationships.

Kinetic predictions concerning the long-term stability of TKX-50

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Keywords: activation energy; TKX-50; kinetic studies; long-term stability; storage safety.

TKX-50 is one of the most promising candidates for RDX replacement over the last decade. Therefore, it is of high interest to investigate the long-term stability of this compound. In this work, TKX-50 was analysed by means of different kinetic models in order to be able to make predictions about its long-term stability. For this purpose, the compound was synthesized according to a literature-known procedure and thermogravimetric measurements were performed. These were analysed using the Ozawa-Flynn-Wall, Friedman and ASTM E698 kinetic models with the NETZSCH Kinetics Neo software and the activation energy and isothermal long-term stability were determined.

Time-temperature superposition applied to PBX damage evolution

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Keywords: PBX; damage; time-temperature superposition principle.

Investigating damage in polymer bonded explosives is necessary to produce safe, reliable, and effective compositions. Previous works on hotspots have shown the effect of defects on initiation and it has long been known that 'explosives become more sensitive with damage', although the exact mechanisms are still poorly understood. A full picture of the effect of damage requires an investigation across the full range of strain rates an energetic could experience in its lifetime. A full range of strain rates can be difficult to achieve experimentally, with most works conducted in the ranges achieved by Universal Testing Machines and Hopkinson Bar set ups. Recent works have begun to investigate the proposition of using the Time-Temperature superposition principle as a proxy for using a range of strain rates in the mechanical testing of energetic materials. However, the effect of changing damage mechanism has yet to be explored. In this work, the response of cubic fine and coarse grained RDX-HTPB samples parallel and perpendicular to damage is investigated. High strain rate loaded samples, achieved using a Direct Impact Hopkinson Bar, are compared to low rate loaded samples. At room temperature, the coarse-grained samples undergo a transition from an anisotropic response at low strain rates to an isotropic response at high strain rates. This can be explained by considering a transition from partial to total debonding. The effect of reducing temperature, at low strain rate, is then investigated in this work. Alongside this, at the strains investigated, the fine grained and bimodal samples exhibited isotropic responses. The effect of lowering temperatures on these samples, and an exploration of the onset of the transition from partial to total debonding, is also discussed.

Preparation and stabilisation of amorphous energetic materials

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Keywords: amorphous; melt-quench; resonant acoustic mixing; TNT; TATB.

Energetic materials (EMs) are traditionally studied in their crystalline form, however, the material properties exhibited by the amorphous state can offer significant advantages, such as decreased sensitivity to impact initiation. Amorphous EMs are therefore less likely to be prone to accidental detonation. In this work, we have explored ways to obtain and stabilise amorphous solid dispersions (ASD) of 2,4,6 trinitrotoluene (TNT) using melt-quenching and resonant acoustic mixing (RAM) as a milling technique. The degree of amorphisation obtained is assessed by powder X-ray diffraction measurements. Polyvinylalcohol (PVA) and polyvinylpyrollidone (PVP) were successful in creating and stabilising a 1:1 (TNT:polymer) ASD preparation for up to one week at room temperature, while TNT: PVA was also successfully created by RAM milling. These results show that there is definitely potential to store this powerful EM in its amorphous state. 2,4,6-triamino-1,3,5-trinitrobenzene (TATB) was also studied using the RAM milling technique and preliminary results suggested that this compound can be successfully prepared as an ASD which was stable for > 1 week. Overall this research has highlighted very promising avenues for obtaining and stabilising amorphous forms of EMs.

The impact of polymorhism on impact sensitvity - a computational study

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Keywords: impact sensitivity; computational; polymorphism; structure-property relationship; computational screening.

The development of a computational screening programme for new energetic materials not only reduces the inherent danger of working with such materials but also allows for deeper understanding of structure-property relationships. One such relationship which has not been studied in depth experimentally is the effect that polymorphism has on impact sensitivity, even though considerable work has been done to characterise these polymorphs. Here, a predictive tool which accurately predicts impact sensitivity of materials, by modelling the efficiency of shock energy to vibrationally excite high energy molecular modes in crystal structures, is used to predict the impact sensitivity of the known polymorphs of energetic materials including NTO, RDX, HMX and TNT amongst others. This work will not only provide valuable information on the effect that polymorphism has on impact sensitivity but will also discuss the further implications that this has with regards to incorporating crystal structure prediction with the aims to develop a fully computational screening method.

Tailoring the properties of FOX-7 using co-crystallisation

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Keywords: FOX-7; co-crystal; crystal structure; impact sensitivity; hydrogen bonding; energetic materials; 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. 1,1-Diamino-2,2-dinitroethene (FOX-7) is a secondary explosive, that has very low sensitivity to both impact and friction, as well as high explosive performance. This property originates from a combination of substantial delocalisation within the molecule combined with strong intermolecular and intramolecular hydrogen bonding. The co-crystallisation studies of FOX-7 offer an opportunity for understanding the structure-property relationships in EMs. In this research, p-phenylenediamine (PPD) has been selected as a co-former on the base that it may mimic the intermolecular interactions and disrupt the extensive intermolecular hydrogen bonding in FOX-7. A co-crystal of FOX-7 and PPD has been successfully prepared and structurally characterised using single-crystal X-ray diffraction, X-ray powder diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR). The single-crystal study revealed the presence of extensive hydrogen bonding and drastically changes the conformation of the FOX-7 molecule. The impact sensitivity of the new material has been measured using a BAM Fall Hammer and this highlight how the structural changes have a very substantial effect on the impact sensitivity of the new co-crystal.

Research output software for energetic materials based on observational modelling (RoseBoom)

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Keywords: prediction of performance; computer program.

There is huge scope for the implementation of sustainable methods in the research of new energetic materials. It is certainly one of the most important aspects which must be considered and implemented in current and future modern scientific research. There are a number of ways this can be achieved, and with the development of the program "Research output software for energetic materials based on observational modelling"(RoseBoom) it is hoped that the development of new modern energetic materials will be advanced, since it aims to provide access to quick and easy prediction methods which will indicate performance parameters (e.g. the detonation velocity and pressure, the key indicator for the power of an explosive)- before they have been synthesized.

Adjustability of energetic coordination compounds: comparison of three 1-(azidoalkyl)-5H-tetrazole ligands and their energetic coordination compounds

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Keywords: energetic coordination compound; primary explosive; tetrazole; azido-alkyl tetrazole; sensitivity.

Energetic coordination compounds (ECCs) are currently extensively discussed as potential primary explosives to substitute poisoning lead styphnate as well as lead azide in initiation devices. The energetic properties of ECCs are easily adjusted by the selection of different metal cations, energetic anions as well as numerous nitrogen-rich ligands. Three promising ligands which can be used in ECCs are 1-(azidopropyl)-5H-tetrazole (APT), 1-(azidoethyl)-5H-tetrazole (AET), and the highly energetic 1-(azidomethyl)-5H-tetrazole (AzMT). By shortening the alkyl-chain from APT over AET to AzMT the heat of formation, thus the energetic performance of the ligand itself, is drastically increased. While the ECCs containing AzMT belong to extremely sensitive compounds, capable to initiate PETN and hexogen, the comparable ECCs of AET and APT offer a lower sensitivity, thus a safer handling. Here the three ligands APT, AET, and AzMT are compared as well as some corresponding ECCs. Sensitivity values, thermal stability and the result from hot plate and hot needle test, are used in order to demonstrate the great adjustability of energetic coordination compounds.

Ultrasound-induced damage in high solid load polymer-bonded explosives

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Keywords: ultrasound; polymer-bonded explosive; hot spots.

Inducing damage via hot spots in energetic materials provides valuable insights into similar mechanisms during detonation events. Ultrasonic treatment is a potentially interesting damaging method, as ultrasound is capable of causing melting, delamination and decomposition of energetic material single crystals and crystal clusters. Additionally, the heat generated by ultrasound may cause crystals to change state to potentially more sensitive phases. To this point, however, ultrasound has not been used on high solid load materials that are more representative of energetics materials currently in use. This study presents the development of an acoustic treatment method to damage high solid load polymer-bonded explosives (PBXs). A set-up was designed to treat a HMX-based PBX similar to PBXN-110. To tune the set-up and investigate the main damage mechanism, sugar was initially used as a substitute for HMX. Thermochromic pigments were used to gain insight into local heating, which was found to be the main damage mechanism. Results showed that it is possible to reliably achieve temperatures over 180 °C. For the PBX, decomposition of the binder was observed. Moreover, the phase transition from β-HMX to δ-HMX, which has been reported to result in more shock sensitive PBXs, was confirmed visually. Although the developed treatment method affected mostly the surface of the PBX, these results demonstrate the potential of ultrasonic treatment as a method to study damage in energetic materials.

Synthesis of energetic materials using flow chemistry

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Keywords: low chemistry; energetic materials; 2,4,6-TNT; ETN; trace detection; aviation security.

This paper describes the potential of flow chemistry for the safer and more sustainable synthesis of energetic materials compared to traditional batch methods. This on-going work is performed in the frame of the development of explosive standards used by the European Commission and Member States' aviation security inspectors to verify the detection performance of explosive trace detection (ETD) in airports. The motivation to apply flow chemistry for the synthesis of energetic materials was to eliminate the hazards linked to synthesis of explosives using conventional batch methods. Our on-going research involves the synthesis of ETN using flow chemistry, and it follows on from our previously developed method of 2,4,6-TNT synthesis. The advantages of synthesising energetic materials by applying flow-based methods compared to batch methods is discussed.

Evaluation of thermal diffusivity of solid propellants by flash method

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Keywords: solid propellant; thermal diffusivity; flash method; ignition.

Solid Propellants are widely used in a various pyrotechnical devices, including rocket motors and gas generators. Most of these reactive materials exhibit high sensitivity to thermal solicitation. Their interaction and behavior within a pyrotechnic system need an accurate knowledge of thermal properties, like thermal diffusivity, leading to ignition and combustion. From a test facility initially designed to evaluate the ignition and combustion properties of solid propellants, the aim of this study is to determine the diffusivity of a solid propellant by the flash method, taking into account the characteristics and dimensional constraints of the test facility. The flash method is a classical method for determining the thermal diffusivity of a material. The method consists in imposing a brief and intense light flux on one side of the sample and measuring the temperature evolution on the opposite side. Then, the thermal diffusivity of the sample can be deduced by analysing the thermogram. To reach this aim, a numerical study is carried out to evaluate the influence of the various control parameters such as the spatial distribution of the thermal flux, the temporal evolution of the laser pulse, the thermal transfers at the walls, the local rise of temperature and thermal properties within the material, the intrusivity of the thermocouple. Moreover, this design takes into account the experimental restrictions of the test facility as well as the risks of degradation or ignition of the samples.Finally, a test campaign is conducted on a reference composition. The analysis of the thermograms allows us to assess the experimental uncertainties obtained, the performance of the thermal analytical models applied and the relevance of the experimental approach.

Impact and friction sensitivity of acidic PETN

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Keywords: PETN; sensitivity; drophammer; impact; friction.

In order to better assess the hazards associated with the industrial manufacture of pentaerythritol tetranitrate (PETN), a laboratory reactor for the synthesis was developed in cooperation with BIAZZI and Austin Powder. The reaction conditions are as close as possible to the industrial standard. In case of an emergency on a plant, like loss of cooling water or agitator failure, the reaction solution is drowned on water. This scenario was performed in laboratory scale and the mechanical sensitivity of the resulting PETN was investigated. Samples with a content of 0 to approx. 35% of the drowned acid were tested for impact and friction sensitivity. Problems in the accurate measurement of mechanical sensitivities as well as emerging trends in the results are intensively discussed. Knowing those sensitivity data can help to avoid accidents during cleaning and to optimize mechanical components.

Continuous-flow synthesis of dichloroglyoxime

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Keywords: flow chemistry; heterogeneous reactions; dichloroglyoxime; chlorination.

Dichloroglyoxime is an intermediate in the synthesis of the promising energetic material dihydroxylammonium-5,5'-bistetrazole-1,1'-diolate (TKX-50). The classical synthesis by chlorination of glyoxime with elemental chlorine in batch has numerous disadvantages concerning safety and scalability due to the exothermic and heterogeneous nature of the reaction. Because of to the high reactivity of the intermediates and to prevent further chlorination and subsequent decomposition of the product, cooling of the dispersion to -20 řC is demanded. This requires strong cooling capacity and intense mixing, but also poses the risk of thermal runaway and a large toxic inventory. In order to overcome these drawbacks and still utilize the high atomic economy and the low cost of chlorine as a chlorination reagent, a continuous-flow synthesis was developed. The resulting process has decisive advantages for upscaling the synthesis, such as significantly higher reaction temperature and increased safety. The low volume of the flow reactor provides a lower toxic inventory during the reaction compared to a conventional batch reactor. With a lab bench-scale setup a dichloroglyoxime throughput of 31 g/h was achieved with a yield of 70 %, comparable to the batch reaction. Moreover, the reaction temperature in the flow reactor could be increased to 20 řC and the chlorine gas is fed into a closed reaction system and fully conversed.

Predicting the technology readiness level of NTREM papers

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Keywords: NLP; machine learning; energetic materials.

Technology Readiness Levels (TRL) assign a numeric value to the maturity of a technology. Identifying the TRL of novel technology in a journal article is an involved process requiring expert assessment. This work aims to identify and utilise Natural Language Processing (NLP) tools for automatic classification of energetic material journal articles based on their TRL. This problem is explored using a small dataset of New Trends in Energetic Materials (NTREM) articles each with an expert assigned rating of "low" or "high" TRL. Small datasets arise when information is restricted, for instance in sercurity-related or financial fields, and pose problems such as overfitting. This investigation also seeks to explore these issues surrounding the use of small datasets. First a methodology for extracting text from journal articles is described. Then a range of supervised machine learning methods are investigated. To avoid overfitting, various methods are explored such as state-of-the-art transfer learning methods using Bidirectional Encoder Representations from Transformers (BERT). The results are compared to a baseline frequency-based keyword matching algorithm. Results show, even with a small dataset, NLP machine learning methods can categorise NTREM articles into "high" and "low" TRL with an accuracy that outperforms the baseline measures.

Additive manufacture of energetic materials: assessing the printability of energetic composites

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Keywords: additive manufacture; energetics; extrusion; paste.

Recent years have seen a huge growth in the use of additive manufacture in various applications, from simple 3D printing of thermoplastics to more complex processes used to form functional parts. There is now a considerable interest in applications of additive manufacture to energetic materials, such as propellants and explosives, as shape and structure can greatly influence their effect. In developing additive manufacturing tools and techniques applicable to a range of highly filled energetic composites, it would be desirable to develop an understanding of the "printability" of these materials and how this relates to their composition and rheological properties. This talk will present an approach to assessing the printability of energetic composites using methods previously developed to model paste extrusion. In this approach, custom built apparatus is used to assess the extrusion of small samples across a range of conditions in order to extract material specific parameters which can be used to model material flow under a variety of extrusion conditions, including those used in additive manufacturing. Results will be presented in which this methodology has been used to assess inert materials as well as the Extrudable Paste Explosive (EPEx) series of formulations developed by the Defence Science and Technology Laboratory (Dstl). Extrusion models have been built for these materials, allowing for the assessment of different printing process designs. In discussing these results, the potential benefits will be considered, including the ways in which modelling of material extrusion can be used to aid the development of additive manufacturing techniques suitable for highly filled energetic composites.

Development of an automated approach for chemical synthesis knowledge graphs directly from text corpora

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Keywords: natural language processing; information extraction; knowledge graph; retrosynthesis.

Within the last two decades, interest in computationally-assisted synthesis planning as well as natural language processing have increased significantly but separately. As a result of research efforts within these domains, basic tools for information extraction and retrosynthesis and reaction optimization are now openly available. The objective of this work is to explore the intersection of these two emergent research capabilities and develop automatable approaches for extracting chemical synthesis information from text documents to create novel representations via knowledge graphs. Graphs have been used to represent both natural language and chemistry data in disjoint instances. Within this work, natural language processing tools designed for chemistry literature are utilized to extract the synthesis data from text, and then produce that data in a graph database format. The resulting knowledge graph is heterogeneous, combining chemical information along with natural language, primarily molecular and procedural information, including reactants, reagents, products, and reaction conditions. We specifically examine the subgraphs for the synthesis information of several molecules, including 1,5-diamino-2,4-dinitrobenzene, to verify the fidelity and integrity of the information contained within the graph produced by the automated approach. Finally, we examine an approach to predict alternative synthesis ingredients using knowledge graph embedding algorithms to recommend likely substitutes.

Effect of the fuel used on the burning mechanism of nanothermite compositions

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Keywords: nanothermite; pyrotechnic.

Nanothermite compositions demonstrate a number of unusual behaviours, like an high linear burning velocities (even up to 2500 m/s), decrease of burning velocity with a rise of density, low temperature of ignition, short times of burning induction and of development of a stable burning process. An important distinguishing feature of nanothermites is an unusual mechanism of combustion, different from the burning mechanism of micrometer fineness compositions, so far only partially described and poorly explained. Despite the supersonic propagation velocities of high-energy transformation and high pressure rise rates occurring for some nanothermites, these transformations cannot be classified as a detonation process. Among the theories aiming to describe the combustion mechanism of these compositions, one can mention the reactive sintering model or the melt dispersion mechanism (MDM) model. However, these models are not complete because they do not fully explain the phenomena occurring during the burning of nanothermites. One of the key parameters affecting the propagation mechanism of the high-energy reaction is the fuel used in a given system. Changing the fuel, not only leads to a change of the high-energy parameters, but also results in a complete change of the mechanisms regulating their combustion. The aim of this work is to discuss the influence of the applied fuel and its parameters, such as occurrence and parameters of passivation layer, reactivity, melting point etc. on the process of combustion propagation. Also, an objective of this work is to confront the existing theories describing the burning process of nanothermites.

Multiphoton excitation for standoff detection of fuels in plastic containers

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Keywords: laser sensing; standoff detection; ANFO.

The Prescott Environmental Luminescence Laboratory is an Australia Defence Science and Technology (DSTG) linked facility, undertaking research in areas such as sensing for counterterrorism and radiation monitoring. Current projects include the interactions of high-powered lasers with secondary explosives and materials of security concern, towards the goal of standoff detection.

Laser-induced fluorescence is a powerful technique, with rapid discrimination of materials at standoff distances possible if the material in question can be correctly excited and its emission signal collected. While fluorescence detection is often undertaken with UV sources, plastics such as those in PET drink bottles readily absorb UV light, preventing the excitation and therefore detection of their liquid contents. However, our research demonstrates the possibility of using visible light instead of UV for excitation.

Through this technique of excitation using visible to visible multiphoton fluorescence, an anti-Stokes shifted emission is created that can be characterised to both detect and discriminate between various liquid fuels of security concern through clear plastics.

Petroleum products in particular contain large amounts of highly fluorescent polycyclic aromatic hydrocarbons (PAHs). PAHs are a class of fused hydrocarbon ring molecules, ranging from simple naphthalene to large, high molecular weight arene systems. Many of these molecules have distinct emission spectra, so a fluorescence-based system has the potential to optically characterise the PAH content of a target material.

As the range and ratio of different PAHs varies significantly between different types of fuels, we propose that this emission profile can be used to rapidly discriminate between petroleum fuels, including those used for both improvised and commercial grade ANFO mixtures. A fluorescence system could therefore lead to optical fingerprinting of improvised ANFO fuels to determine their origin while remaining at a standoff distance and not physically contacting the explosive, essential criteria for scenarios involving unknown improvised explosives.

Progress towards defining the UK methodology for the stability testing of energetic materials

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Keywords: stability testing.

The UK Defence Ordnance Safety Group (DOSG) provides advice to project teams, the armed forces and industry on Ordnance, Munitions and Explosives (OME). The UK needs to maintain research into new energetic material technology. As the UK's inventory is increasingly procured from non-UK sources, it has become essential to understand testing and evaluation undertaken in the country of manufacture. It is vital to align UK testing with that of other NATO allies, whilst maintaining the UK database of knowledge to ensure continued OME safety.

In 2019, a programme of work was started to understand the stability of a selection of gun propellants using a number of techniques including accelerating rate calorimetry (ARC), the mass loss test and heat flow calorimetry (HFC). One of the aims of this programme was to define the reproducibility of the techniques and to understand the variability of the results which have been observed previously for such materials.

This paper discusses the ARC, mass loss and HFC data from three gun propellants which were used in this study. The results demonstrate that the HFC data were highly consistent and it supports the continued used of this technique for such materials. However, the information gained from the mass loss test in its current form appears to be more limited in value. Additionally, there are a number of issues with respect to the use of ARC for understanding the stability of gun propellants and discussions around this are the focus of this paper.

A computational study of ballistic modifiers in the fizz reaction zone of double base propellants

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Keywords: Pb ballistics; double-base propellant; DFT; carbon matrix; adsorption.

Ballistic modifiers are additives in double base propellant (DBP) formulations which modify the burning rate of the propellant to pressure and initial temperatures. Lead-based ballistic modifiers are widely used due to their plateau-burning characteristics, producing a steady fuel burn rate. However, incoming European legislation will soon ban their use, and modifiers based on other metals fail to replicate the burn-rate profile offered by lead.

This computational study focuses on the prominent carbon soot theory for catalysis, where lead-based particles (from their decomposition) are catalysts at the burning surface embedded in a carbon matrix. The formation of this lead/carbon matrix is responsible for initial catalysis of the burn rate, and its subsequent loss at higher pressures determines the plateau mechanism.

Through the investigation of small lead oxide clusters that could form in the gaseous zone near the burning surface, it has been demonstrated that the addition of small amounts of carbon rip apart the clusters. The resulting carbon matrix, dispersed with exposed metal sites, forms the burn rate catalyst, which acts as a Lewis acid to bind small molecules such as NO2 in the combustion flame. We also highlight the importance of very weak Pb-C bonds, which suggest that Pb atoms are unlikely to be retained in the carbon matrix that forms in the combustion flame.

Optimization of thermobaric explosives formulations by numerical modeling of detonation

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Keywords: thermobaric explosive; detonation; numerical modeling; EXPLO5; XW; semi-empirical method.

The development of high-performance thermobaric or enhanced blast explosive compositions (TBXs or EBXs) is one of the most prominent trends in new technologies of explosives, due to their high destructive effects compared with conventional weapons. When designed and manufactured in form of plastic bonded explosive (PBX), thermobaric compositions consist of a high explosive , usually a nitramine, reactive metallic powder, an oxidizer and a polymer binder. The thermobaric effect is a combined effect of the shock wave in the air and a high amount of released heat during the explosion. Numerical models can save resources for research and development and reduce the risks of extensive experimental work.

This paper presents a study of characterization and optimization of specific TBXs formulations by the means of numerical modeling using EXPLO5 thermodynamic code, XW soft-ware, and the Jeremić-Bogdanov semi-empirical method. Numerical modeling was used in order to analyze influence of individual components in TBX formulations on parameters of detonation and thermal effect. For the selected thermobaric explosive compositions, the calculated parameters were compared with experimental results in order to confirm the applicability of used numerical models. Correlations were drawn in direction of future approaches for optimization of TBX formulations.

Application of thermochemical computer code in the prediction of nano-scale nitramines performance

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Keywords: nano-nitramines; EXPLO5; RDX; HMX; CL-20; velocity of detonation.

The nanotechnology approach, in the field of explosives, is known to lead towards re-duced sensitivity, improved performance, and enhanced safety. Downsizing energetic materials particles to nano-scale modifies their structure which in turn positively affects the overall explosive properties. However, any experimental research involving nano-sized energetic materials is costly and often highly hazardous. Therefore, numerical mod-elling and computational prediction of the velocity of detonation and other energetic properties would be valuable before initiating any laboratory tests. The present work has examined and demonstrated the possibility of applying the computational modelling by the thermodynamic code EXPLO5 to estimate the energetic performance of nano-nitramines and compositions thereof. Simulation is conducted on the most studied ni-tramine explosive compounds (RDX, HMX, and CL-20), at both nano and submicron particle size, when incorporated in explosive charges (PBX and booster) and propellant. EXPLO5 was run at a mode suitable for nano-particles then the obtained results were compared to already known experimental values of energetic performance parameters.

In-situ characterization of solvent mediated cocrystallization of HNIW/HMX

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Keywords: FBRM; PVM; co-crystal; HNIW; HMX.

Solvent mediated cocrystallization is one of the promising technique for preparation of 2:1 cocrystals of HNIW and HMX in the view of process simplicity, scale-up, product quality, crystal growth control and yield. Various studies conducted in recent years that focused the final product characteristics but the formation of the cocrystals still need some attention. In this study, solvent mediated cocrystallization of HNIW and HMX studies conducted with different solvents with FBRM (Focused beam Reflectance Measurement) and PVM (Particle View Measurement) probes as in-situ characterization method, to understand and observe the formation of cocrystals and crystal growth. In addition, samples taken at different periods during cocrystallization and subjected to XRD and SEM analyzes. The final product was also characterized by particle size, density, impact sensitivity, friction sensitivity, vacuum stability, DSC, TGA and HFC.

Boron-based thermobaric explosive computational modeling and possible optimization paths

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Keywords: boron; thermobaric explosive; PBX; polymer binder; EXPLO5.

Due to its high gravimetric and volumetric heat of oxidation, elemental boron powder is one of the best candidates for metal fuel components of thermobaric PBX, along with beryllium and aluminum. Besides the high ignition temperature of boron, there is another drawback to its application low compatibility with the most often used polymeric binder, HTPB. When added to this binder, boron causes a rapid increase in the viscosity, resulting in practically uncastable consistency of the mixture. This research examines the possibility to optimize TBE compositions in thermodynamic code EXPLO5, by replacing HTPB with another polymeric binder. The velocity and heat of detonation were determined and compared with experimental results for a chosen thermobaric composition, HMX/AP/Al/Mg/B/HTPB. Predicted performance parameters were discussed for the proposed optimized compositions.

The structural combination of TKX-50 and MAD-X1: synthesis and characterization of 5-(3-Nitro-1,2,4-triazol-1-ol-5-yl)-tetrazol-1-ol

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Keywords: energetic materials; X-ray diffraction; tetrazole; triazole; secondary explosive.

With the synthesis of 5-(3-nitro-1H-1,2,4-triazol-1-ol-5-yl)-1H-tetrazol-1-ol we can report the first successful production of a structural combination of the heterocycles tetrazol-1-ol and triazol-1-ol. The obtained hybrid product resembles one half each of the established energetic bis-heterocyclic compounds dinitro-bis-(1,2,4-triazole)-1,1'-diol and 5,5'-bistetrazol-1,1'-diol on which the explosives TKX-50 and MAD-X1 are based on. The straightforward synthesis modifies the cyano moiety of the cyano-nitrotriazole starting material to the tetrazol-1-ol within 3 reaction steps. The selective N-oxidation of the triazole to the triazol-1-ol was achieved in a fourth and final reaction step using Oxone® under specific pH and reaction parameters. In order to tune and improve the performance parameters, several nitrogen rich bases were used to obtain the respective ionic derivatives including the ammonium, hydrazinium, guanidinium, aminoguanidinium, triaminoguanidinium and the hydroxylammonium salts. All compounds were characterized using multinuclear NMR and IR spectroscopy, differential thermal analysis (DTA) and elemental analysis. Several compounds could be further analyzed using X-ray diffraction measurement. The heats of formation for all investigated compounds were determined and the detonation properties (EXPLO5 V6.05.02) were calculated. These data, as well as the sensitivity values were compared to related substances.

Influence of diameter of explosive charge and thickness of steel confinement on detonation velocity of ANFO explosives

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Keywords: ANFO; velocity of detonation; steel confinement.

Due to its satisfactory effect during blasting, technical and detonation properties, and relatively low prices, ANFO explosive is mostly used in mining and construction works. In addition to the economic factor, other reasons for its frequent use are safety during blasting, ease of on-site production, and the possibility of filling boreholes by machines. The paper presents the measurements used to determine the influence of the diameter of explosive charge and the thickness of the steel confinement on the detonation velocity of the ANFO explosive.

Energetic azoxy compounds as crystallization modifiers in melt-cast explosives

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Keywords: melt-cast explosive; 2,4,6-trinitrotoluene; 2,4-dinitroanisole; crystallization modifier; azoxy compound.

Melt-cast energetic compositions containing 2,4,6-trinitrotoluene (TNT) or 2,4-dinitroanisole (DNAN) are well-known and widely-used. An important stage in the production of munition is the solidification process of compositions containing these explosives. The addition of a crystallization modifier allows to avoid the creation of caverns in the castings. The effect of various modifiers on the crystal growth of TNT or DNAN samples were investigated. The following compounds were used as crystallization modifiers: azoxytetranitrotoluene, azoxytriazolone, diaminoazoxyfurazan. Polarized Light Microscopy was used to determine the structure of obtained crystals. The density and hardness of obtained samples were also tested. TNT and DNAN castings with hexanitrostilbene (HNS) and without additional modifier were selected as references.

Synthesis, characterization, and functional group substitution of energetic triazines

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Keywords: heterocycle; 1,2,4-triazines; amination; oxidation; energetic materials.

Energetic materials (EMs) are used in military and commercial applications across the globe. These materials need to be storable, transportable, and effective while remaining environmentally safe. A good EM should have high performance capabilities while being insensitive to stimuli, thermally and chemically stable with simple and inexpensive to synthesis routes. The reaction of diazotetrazole with nitroacetonitrile is a straightforward synthesis for the single-step formation of energetic 3-azido-5-amino-6-nitro-1,2,4-triazine. Reduction of the azide via a modified Staudinger reaction readily yielded 3,5-diamino-6-nitro-1,2,4-triazine which was oxidized using potassium peroxymonosulfate triple salt (Oxoneő). Chemical characterization of these triazines was performed by Nuclear Magnetic Resonance (NMR), mass, infrared (IR) spectroscopy, and elemental analysis. Single crystal X-ray crystallography was used to determine molecular structure and density. Energetic sensitivity to impact and friction were determined using a OZM Drophammer and BAM friction tester and thermal stability of the material was determined by differential scanning calorimetry (DSC) or thermal gravimetric analysis (TGA). Gaussian09 was used to calculate the solid-state heats of formation while the detonation parameters at the CJ point and oxygen balance were calculated using EXPLO6.05.

Solvent free polyurethanic binders for pyrotechnic compositions

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Keywords: pyrotechnic; polyurethane; safety; polyol.

This paper describes the investigations related to the development and characterization of various plastic pyrotechnic compositions based on polyurethane binders synthesized from commercial isocyanates and polyols obtained by the catalytic degradation of recycled PET (polyethylene terephthalate). These types of binders improve the processability and minimize the risk associated with the manufacture process. A comparative experimental study was performed between these newly developed pyrotechnic compositions and the conventional ones, in order to establish the improvements that could be made, in terms of safety and performance.

Trinitro-Orcinol (C7H5N3O8) as anion in energetic metal compounds

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Keywords: energetic coordination compound; primary explosive; sensitivity.

Energetic coordination compounds (ECCs) are currently under investigation as new primary explosives as well as ingredients in pyrotechnical compositions. Trinitro-orcinol (TNO, 1,3-dihydroxy-5-methyl-2,4,6-trinitrobenzene) was prepared by nitration of 5-methyl-resorcin (orcinol) in mixed acid. The neutral compound is compared to styphnic acid. Several energetic coordination compounds were synthesized by combination of different metals, high-nitrogen ligands and TNO. The new ECCs were compared to known styphnate derivatives and characterized intensively by low temperature XRD, vibrational spectroscopy, thermal analysis, elemental analysis and sensitivity measurements.

Thermal, calorimetric and morphologic characterisation of polyuretane based composite flare pyrotechnic material

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Keywords: polyurethane; composite; flare; chlorinated rubber.

The use of poymeric binders for pyrotechnic compositons is used extensively in the last decades, given the advantages regarding their mechanical strength, resistance to humidity and their relative good chemical stability. The use of solvent free polyurethane formulations binders have the advantage that big, compact geometry grains can be obtained and also the manufacturing process is facile and safe, by using squeeze casting method. The main disadvantage of this polymeric binder is related to the inhibition of the burn rate, when used in conjunction with oxidants like potassium perchlorate or fuels like aluminum of aluminum-magnesium alloy. This paper presents the thermal (DTA), calorimetric (heat of combustion and specific volume), burn rate and flame temperature of a composite pyrotechnic mixture based on combined binder comprising polyurethane and chlorinated rubber. The use of chlorinated rubber in the composition greatly improves the burn rate and flame temperature, while the other parameters measured are comparable to polyurethane based compositions. While the theoretical calculation made with Explo5 software do not predict an important increase in the calorific properties of the material, the SEM-EDS investigations show a very effective mixing of oxidant-chlorinated rubber-fuel matrix, that explain the dramatic burn rate increase. This finding could prove valuable in designing flare pyrotechnical compositions and compositions in an cost effective manner and with an extended estimated service life.

Direct alkylation of nitroguanidine by reaction with alkylamines – investigation of reactivity and optimization

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Keywords: alkylnitroguanidine; nitroguanidine derrivative; melt-cast explosive; synthesis optimization.

Alkylnitroguanidines are compounds known for almost 100 years. Recently they have attracted considerable interest as prospective ingredients of melt-cast explosive compositions exhibiting reduced sensitivity to mechanical stimuli. This is mainly due to the low cost of obtaining them in the reaction of direct alkylation of nitroguanidine with aliphatic amines. This reaction, also known as transamination, is done in a single step, and uses only non-expensive, widely available substrates. Moreover, it takes place in an aqueous environment and does not require catalysts, therefore it also meets the criteria of green chemistry. This work presents the observations and conclusions on the transamination reaction of nitroguanidine, gathered during the optimization work on the synthesis of several different alkyl derivatives. The investigated compounds differ not only in the length of the carbon chain, but also in its branching or the presence of unsaturated bonds. The influence of temperature, reaction time and the molar ratio of the reactants on both the yield and purity of the obtained product were investigated. The reaction scale-up process was also conducted. The test results show that with appropriate selection of the reaction conditions it is possible to reliably obtain alkyl derivatives in high purity and with good yield.

Detonation performance of urea hydrogen peroxide

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Keywords: urea hydrogen peroxide; detonation; non-ideal explosive; performance.

Carbamide Peroxide is commonly used in the cosmetic and pharmaceutical industries as a solid source of hydrogen peroxide. This adduct of Urea and Hydrogen Peroxide (UHP) has explosive properties, which have been only recently studied, highlighting its behaviour of non-ideal tertiary explosive and detonability at large scale. Our work focussed on investigating UHP detonability in the 100 g-scale. A maximum of experimental data, collected from combining laboratory and underwater measurement campaigns, is required to evaluate the detonation performance of non-ideal explosives. Our lab results confirmed self-sustained detonation under heavy confinement, with observed detonation velocities consistent with literature values from large-scale field experiments. We further fired UHP charges underwater and quantified brisance and explosive power respectively from underwater shock pressure and bubble period. By comparing experimental results and numerical simulations, we could assess the level of agreement between lab and underwater detonation performance parameters.

Predicting the impact sensitivity of two possible lead azide replacements

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Keywords: sensitivity prediction; computational analysis; lead azide; DFT.

Energetic materials (EMs) are renowned for their ability to release a significant amount of energy upon detonation (the energetic performance) which is tensioned against their sensitivity (the likelihood of detonation when exposed to a given stimulus). Lead azide is a primary energetic which has both high energetic performance and is exceptionally sensitive to impact. The combination of these properties has resulted in it becoming a widely used detonator for more powerful secondary EMs. However, lead-based compounds have many adverse environmental effects, and incoming REACH legislation will limit their use. For these reasons, more sustainable replacements that can match lead azide for energetic performance are sought. The synthesis and characterisation of novel EMs is an inherently dangerous process, however, making the computational prediction of sensitivity an attractive alternative. In this work, lead azide and two potential replacements, based on copper, DBX1 and DBXX2, are investigated computationally using plane wave DFT calculations to ultimately predict and rationalise their impact sensitivities using a vibrational up-pumping model. The predicted impact sensitivity values exhibited excellent agreement with experimentally determined sensitivities, and gives insights to rationalise the origin of their high sensitivity. This fully computational approach provides an attractive alternative to dangerous experimental work, and also offers a design tool to explore and create EMs with tailored energetic properties.

Melt crystallization of ammonium dinitramide suspensions with additives investigated by means of X-ray diffraction

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Keywords: ammonium dinitramide; melt crystallization; X-ray diffraction.

Ammonium dinitramide is a promising oxidizing agent for solid rocket propellants. In-situ XRD investigations of ADN suspensions with different additives are performed to understand emulsion crystallization processes of spherical ADN particles (prills). Therefore, samples are heated to the melt at 96 řC in an X-ray diffractometer and cooled stepwise to room temperature. Diffraction patterns, captured after the temperature steps, are evaluated in terms of crystallinity and microstructure. The investigations reveal significant differences of the crystallization behavior of ADN suspensions and show the influence of additives and liquid media. The results shall be used to improve the quality of ADN prills, e. g. produced at the Fraunhofer ICT technical plant.

The study on the crosslinking and curing of poly(glycidyl azide) (GAP)

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Keywords: GAP; isocyanate; cross-linking; propellant.

The study on the crosslinking and curing of poly(glycidyl azide) (GAP) with commercially available isocyanates was conducted. Bifunctional isocyanates, trifunctional isocyanate, two types of catalyst, chain extender and linear bifunctional GAP were used in this study. As a result of the research work on GAP crosslinking, several systems were selected to propellants. The best results were obtained for polyurethanes obtained from the combination of a trifunctional isocyanate and GAP. Pre-crosslinking of the sample was visible already after 48 hours. The use of a catalyst in this system reduced this time to less than 24 hours. A mixture of di- and tri-functional isocyanates is optimal for future mechanical properties. Studies have shown that this isocyanate cures GAP quickly and without additional blemishes in the form of distorted surface or gas bubbles. The compositions of trial batches of propellants with GAP as binder were developed. Different types of crosslinking systems containing isocyanates as curing agents were used. Two different fractions of ammonium chlorate(VII) were used as oxidant. The first with a crystal size of about 200 ţm and the second ground with a fineness of about 20 ţm. The ratio of the two AP200/AP20 ammonium chlorate(VII) fractions was about 3. Plasticizer and bonding agent were used as process additives. All propellants compositions had similar ratios of solid components. The liquid components differed due to different crosslinking systems. Investigations of crosslinking of the obtained polymer allowed to test various types of crosslinking systems containing isocyanates and additives such as chain extenders or catalysts. Depending on the propellant composition and curing system used, propellants with different physico-chemical properties were obtained. The research indicated a further path for the development of fuels based on GAP as a binder. They confirmed the energetic properties of GAP as an energetic binder for rocket propellants.

Preparation and characterization of the butacene based composite propellants

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Keywords: composite propellant; butacene.

This paper presents the characterization of Butacene based composite propellants prepared to obtain enhanced burning rate with low pressure exponent. For this purpose, various HTPB-AP based propellant compositions were prepared by altering solid loading, catalyst amount, oxidizer coarse/fine ratio and amount of burning rate modifiers. Ballistic, mechanical and rheological analysis of the developed propellants were compared. As a result of ballistic analysis, high performance rocket propellants having increased burning rates up to 40 mm/s at 80 bar with pressure exponent around 0,35 were reported. Mechanical and rheological analysis showed poor performance compared to ballistic properties. Nevertheless, despite offering relatively poor mechanical performance, use of Butacene can be considered as a valuable tool to obtain high burning rate propellants. Thus, it would be applicable to trade between mechanical and ballistic properties to some extent according to the desired propellant requirements.

Towards the phlegmatizing of TATP: influence of vacuum oils on its sensitivity to impact and friction

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Keywords: triacetone triperoxide; phlegmatization; impact sensitivity; friction sensitivity.

Triacetone triperoxide (TATP) belongs to the class of organic peroxide explosives and is highly sensitive to mechanical impulses. It can be synthesized from easily available precursors and can be therefore used as improvised explosives. By consequence, these organic explosives are frequently the subject of disposal procedures performed by EOD teams worldwide. The risks during the disposal procedure are due to the high brisance and high sensitivity of the explosives. Using a method to decrease the friction and impact sensitivity of TATP will decrease the risk during the disposal procedure. Currently, the phlegmatization of TATP is often performed using fuel-oil. In our work, it is shown that if fuel-oil decreases the sensitivity to friction of TATP, it is not the case for its sensitivity to impact. One possible explanation for this phenomenon is that gaseous bubbles could be trapped in the mixture and could act as hot spots. Therefore; it was tested to replace fuel-oil by vacuum oil. In fact, the gas solubility in vacuum oil is very low which makes this product category a good candidate for the phlegmatization of TATP. The sensitivity to impact was significantly lower with the vacuum oil than with Diesel. In a second step, the sensitivity to friction of TATP mixed with vacuum oil was tested and compared with the sensitivity of TATP mixed with Diesel. As the vacuum oil permitted to obtain a lower sensitivity, different vacuum oils were tested. The purpose of this screening is to select a vacuum oil which permits to phlegmatize TATP and has a low viscosity which facilitates the phlegmatizing process by the EOD teams. After the selection of a vacuum oil, in a third step, the selected oil is tested on different types of TATP (different crystal sizes and morphologies) to assess the effectivity of the phlegmatizing procedure.

Preparation and properties of some polynitroaromatic compounds containing nitroamino groups

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Keywords: energetic materials; nitroaromatic; nitramines; synthesis; properties.

Several nitroaromatic compounds, tetryl analogs, containing both C-NO2 and N-NO2 groups were synthesized and their properties were investigated. Computer calculated energetic characteristics show that the new EMs possess a perfect values, which are superior in comparison to the TNT. The synthesized compounds were characterized on the basis of HPLC-MS, spectroscopic methods and thermal analysis. Experimental data demonstrate a good thermal stability of investigated materials. Obtained characteristics show that proposed nitroamino compounds can find an application as a secondary high energy materials.

Modern method for crater volume evaluation

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Keywords: crater test; crater volume; 3D scanning; photogrammetry.

Detonating an explosive below a ground level produces a crater in the soil. In an ideal case the crater may have a symmetric conical shape. However, based on the soil type or presence of rocks or other inhomogeneities, the resulting crater may have an irregular shape. In such a case the volume calculation using a simple method by hand measurement with meter traditionally applied may not provide sufficiently precise results. The use of a drone for the 3D scanning makes the technique applicable for evaluation of any size of crater which makes the method suitable for explosivet's evaluation as well as for non-intrusive documentation of effects of accidental explosions. Our work presents a modern method for the crater volume evaluation by drone-based photogrammetry. The crater is firstly 3D scanned, photographs converted to 3D model and volume of the crater evaluated.

Tracking acceleration of projectiles using Photonic Doppler Velocimetry

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Keywords: gun barrel; velocity; internal ballistics; PDV.

One of the important issues in internal ballistics is a relation of chamber pressure to projectile velocity. In a gun barrel, the projectile gradually accelerates until it exits the muzzle end. The muzzle velocity can be measured easily but the acceleration phase is quite difficult to observe. In this paper, photonic Doppler velocimeter was used to track projectiles inside gun barrels. The projectiles were accelerated using 4.5 mm calibre compressed gas gun and 7.62 mm calibre powder gun. Complete velocity profiles have been obtained for gas gun projectiles. In case of powder gun tests, only very short profiles showing initial motion of the projectiles were recorded. Problems associated with this kind of measurements are discussed.

OPTIMEX: First attempts in detonation temperature measurements

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Keywords: optical fibre; pyrometer; brightness temperature; nitromethane.

Electromagnetic radiation in the visible and infrared spectral regions is emitted by detonation waves. This radiation can be used to measure the detonation reaction zone temperature using high speed pyrometers. In this paper, various attempts are shown to capture the detonation light in a way that would enable the temperature measurement using OPTIMEX light analyser. Single and double band pyrometers were built and tested with different types of optical cables and probes using explosive charges of ammine-sensitized nitromethane. High temperature calibration of the dual band pyrometer was performed using a stabilized tungsten lamp and compared to direct sunlight signals. The measured detonation temperature of nitromethane agrees well with available literature values.

Synthesis of 1,3-bis(2-nitroxyethyl)-1-nitrourea and 1,3-bis(2-nitroxyethyl)-1,3-dinitrourea

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Keywords: 1,3-bis(2-nitroxyethyl)-1-nitrourea; 1,3-bis(2-nitroxyethyl)-1,3-dinitrourea.

1,3-bis(2-Nitroxyethyl)-1-nitrourea and 1,3-bis(2-nitroxyethyl)-1,3-dinitrourea as intermediates for energetic materials were synthetized by nitration of 1,3-bis(2-hydroxyethyl)urea. The compounds were characterized by infrared and Raman spectroscopy, nuclear magnetic resonance, differential thermal analysis and elemental analysis. Sensitivity to impact was determined by BAM test. The product may be hydrolysed to produce (2-nitroxyethyl)nitramine.

Comparing long-term stability predictions of commonly known secondary explosives

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Keywords: activation energy; energetic materials; kinetic studies; long-term stability; storage safety.

Explosives are used in both military and civilian applications all over the world. Sufficient longevity and good thermal stability are therefore essential for safe handling and safe storage of energetic materials. In this work, four commonly known secondary explosives, were investigated by means of the Friedman method to be able to make predictions about their long-term stability. For this purpose, the compounds were synthesized according to literature-known procedures and thermogravimetric measurements were performed. Using the NETZSCH Kinetics Neo software these compounds were analysed in regard to their activation energy and isothermal long-term stability.

Structural clarification and characterization of a metal-free primary explosive based on 4-amino-2,3,6-trinitrophenol

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Keywords: primary explosive; nitrophenol; structure eludication; sensitivity; energetic parameter.

During our efforts to evaluate metal free primary explosives, we investigated the diazotization product of 4 amino-2,3,6-trinitrophenol. The latter was first prepared in 1909 by Meldola et al., who falsely recognized this compound as 4-amino-2,3,5-trinitrophenol, also assumed in the Russian literature of the late 19th century. Herein, an optimized synthesis for the obtained nitrophenol was presented and its actual constitution proven by extensive characterization. Furthermore, the diazotization product was prepared and characterized as a metal-free primary explosive. Its energetic properties were evaluated and compared to those of DDNP (2-diazo-4,6-dinitrophenol), which shows poor initiating ability and thermal stability.

Burn rate, combustion heat and flame temperature measurements for metal powders and alloys used in composite energetic materials

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Keywords: burning rate; flame temperature; boron; aluminium.

Metallic powders (Aluminium, Boron, Magnesium, Titanium) and their alloys (Magnesium - Aluminium and Magnesium-Boron) are used in energetic materials as fuels both in pyrotechnic compositions or thermobaric explosives. This paper presents the experimental measurements and theoretical calculations regarding the burn rate, heat of combustion and flame temperature of some pyrotechnic composition based on potassium perchlorate - paraffin - metal powders. The burn rate and flame temperature was measured in atmospheric conditions using a ultrafast infrared camera while the heat of combustion was both calculated using Explo5 Software and determined in oxygen and inert gas using a detonation calorimeter. SEM-EDS analysis was performed on the powders used in the experiments, in order to determine the mean dimension, morphology and the oxide layer thickness. The analysis performed by SEM-EDS and the combustion and flame temperature measurements show a relation between the morphology, mean particle dimension and the burn rate. Flame temperature is not influenced by the burn rate, being related to the chemical composition of the powder or the alloy used in the pyrotechnic mixture. A dramatic increase in the burn rate is observed when the amorphous Boron powder with 5 micron mean size is used in the composition, in place of same mean dimension Aluminum particles. This results is in good agreement with experiments performed with Mg-B and Mg-Al alloys in the same pyrotechnical formulation. The obtained results are of use for selecting proper candidates for fuel components in composite energetic materials, especially those that have polymeric binders that cause a unsatisfactory burning rate.

Towards a crystal structure for nitrocellulose

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Keywords: nitrocellulose; XRD; structure.

Nitrocellulose (NC) is an energetic polymer and the major component of double based propellants (DBPs), alongside nitroglycerin. The stability of NC-based solid propellants, along with their favourable oxygen balance and smokeless burning properties, makes them common amongst rocket launch systems and gun and mortar propellants. Despite the original DBP formulation being over 150 years old, it is still the basis for current formulations. Improvements to tend to focus on the development of additives to enhance material stability and burn-rate properties (1). However, further development and improvements have been hindered by a lack of fundamental characterisation of DBPs, namely the main structural component, NC. Added pressure from the imminent REACH legislation requiring the removal of common lead burn rate modifiers, means a structural understanding of NC has become an even more urgent topic. While there has been some early work on characterizing NC, notably by Miles and Craik in 1930 using X-ray diffraction, the analysis of the data extends no further than suggesting a unit cell. This work, therefore, has looked to prepare highly crystalline NC with a view to characterising it using single crystal X-ray diffraction techniques.

(1) Austruy, H. CHAPTER 9 - Double-Base Propellants; Davenas, A. B. T.-S. R. P. T., Ed.; Pergamon: Amsterdam, 1993; pp 369–413. https://doi.org/10.1016/B978-0-08-040999-3.50014-X (2) Miles, F. D.; Craik, J. Structure of Nitrated Cellulose II. J. Phys. Chem. 1930, 34, 2607. https://doi.org/10.1021/j150317a013

Experimental vapor pressures of 3,5-dihydroxy-2,4,6-trinitrotoluene (TNO) via transpiration method supported by the quantitative HPLC

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Keywords: energetic materials; polynitroaromatic compound; transpiration method; HPLC; vapor pressure.

Polynitroaromatic compounds are important and well-known high-density energetic materials. The substance 2,4,6-trinitrotoluene (TNT), which is often used as a reference, belongs to this class. Another representative of this class is 3,5-dihydroxy-2,4,6-trinitrotoluene (TNO), which can be synthesized with inexpensive and conveniently available reagents.[1] Although TNO can be synthesized in a straightforward way, no energetic, thermodynamic and detonation characteristics are available in the literature. In the absence of such data, an assessment of the safety risks from the use of this substance cannot be reliably performed. In this work the energetic properties and detonation parameters of TNO are determined like described elsewhere.[2] The experimental thermodynamic properties, such as vapor pressures, were determined by collecting the material using transpiration method at different temperature points and quantified by HPLC, resulting in a set of p-T data. The p-T dataset was used to determine a fitting equation based on the Clausius-Clapeyron equation and the p-T data was extrapolated to yield vapor pressures at 298.15 K. The corresponding thermodynamic properties, including molar enthalpy of sublimation, were determined.

[1]: Marchand, A.P. and G.M. Reddy, Improved Synthesis of 3,5-Diamino-2,4,6-trinitrotoluene. Synthesis, 1992. 1992(03): p. 261-262. [2]: Benz, M., et al., Evolving the Scope of 5,5'-Azobistetrazoles in the Search for High Performing Green Energetic Materials. European Journal of Organic Chemistry, 2021. 2021(30): p. 4388-4392.

Determination of camphor concentration profile in deterred single base propellant 5/7SFL

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Keywords: propellant; deterrent; camphor; pirocxilin; raman spectra.

The paper presents the determination of the concentration profile of camphor in a 5/7SFL deterred single based propellant by using Raman microspectroscopic method. Research results show that camphor content on the external surface of propellant grains is 19%, this value decreases by the depth and reaches a thickness of 100 μm. In addition, unlike immersion technology, there is no deterrent on the inner surface of the perforations of propellant grains when using the spraying method.

Preparing and properties of ecological pyrotechnic compositions

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Keywords: pyrotechnic compositions; ecological; REACH; ammunition.

Alteration of pyrotechnic compositions is highly topical today especially in view of the strict REACH legislative, when all temporary exceptions are coming to its end. It is therefore necessary to replace toxic substances used in explosives. These are mainly compounds containing lead, barium and chromium. New materials based on boron, bismuth, molybdenum, but also hydrocarbons have been tested as potential substitutes. The prepared "green" pyrotechnic compositions are following all the environmental requirements, while maintaining physical and functional properties. They have been subjected to the strict assessment and testing in accordance with the relevant ammunition regulations (AOP and STANAG). Special attention was paid to studies of the thermal stability and function in critical situations.

The effect of accelerated ageing on the mechanical properties, chemical composition and morphostructure of a HTPB-AP-Al rocket propellant

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Keywords: accelerated ageing; composite propellant; reticulation density; antioxidant; plasticiser.

Composite rocket propellants based on Ammonium Perchlorate (AP), Aluminium (Al) and Hydroxi terminated polybutadiene (HTPB) are used extensively in both start motors and sustaining motors of medium and large caliber air to air missiles and surface to air missiles. The advantages of this type of composition over the nitrocellulose based double based propellants are related to their greater energetic output and chemical stability. The main disadvantage of the use of HTPB matrix as a binder in the propellant is related to the tendency of the material to develop fracture and cracks, especially when the grain undergoes mechanical solicitations (vibration) at cold temperatures, specific to high altitude supersonic flight. This effect of fracture can have disastrous results, like rocket motor explosion when the propellant is ignited. The effect of aging to the propellant grain is a complex process and is related to the oxidation of the polymer in the presence of AP, the over cross linking of the material and the migration of the plasticizer to the extremities of the grain. The paper presents the mechanical and chemical analysis made on a air to air missile rocket propellant both in environmental conditions and after undergoing an accelerated aging process for 6 moths at 70^0C. Uni axial elongations tests were performed, and the durity of the material was determined. The density of reticulation was analyzed at different time intervals within the ageing process. The plasticizer and the antioxidant depletion was observed by HPLC-PDA analysis. The result corroborates the depletion of the antioxidat with the modification of the reticulation density, the Shore durity and the elongation at break determinations.

Synthesis and emphasized study of TATB/nitramines cocrystals via coagglomeration method

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Keywords: nitramines; co-crystal; coagglomeration; impact sensitivity; intermolecular interactions.

The co-coagglomeration has been used for preparation of energetic material of TATB with RDX, HMX, BCHMX and CL-20, this method has shown advance improvements in the properties of these energetic materials. Molecular rearrangements have been observed employing through characterization methods by Raman, FTIR, and PXRD methods. The significant stretching vibrations indicated that the resultant co-agglomerates (CACs) are cocrystals (CCs). Where HMX is shown in its δ-modification and CL-20 in its β-modification. The differential thermal analysis shown that the stability of these CCs has been relatively same as pure forms these energetic materials. A possibility of the co-crystal formation during co-agglomeration is confirmed by correlations between thermochemical and impact-sensitivity features and various Raman and FTIR outputs. A fresh perspective on the study of co-crystals has been gained by examining these interactions. The co-agglomerates formed have crystal densities very close to their calculated theoretical maximum density.

The influence of Catocene on properties of heterogeneous solid rocket propellants with reduced quantity of HCl in combustion products

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Keywords: solid rocket propellant; burning rate; catocene; combustion.

The aim of this work was to examine how Catocene as a burn rate modifier, impacts on properties of heterogeneous rocket propellants, which contain scavenger compound and emit low amount of HCl during combustion. Usually burn rate modifier is added to propellant slurry in amount approximately 1% of propellant mass. During this work the amount of Catocene was increased to 4.5%mas with the decreasing amount of binder. Seven samples of propellants were made, which had different quantity of Catocene. Mechanical and ballistic properties, sensitivity to friction and impact and isochoric heat of combustion were determined.

Assessing the trade-off between prediction accuracy and interpretability for topic modeling on energetic materials corpora

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Keywords: energetics; machine learning; topic modeling; interpretability.

As the amount and variety of energetic research increases, machine aware topic identification is necessary to streamline future research pipelines. The makeup of an automatic topic identification process consists of creating document representations and performing classification. However, the implementation of these processes on energetic research imposes new challenges. Energetic datasets contain many scientific terms that are necessary to understand the context of a document but may require more complex document representations. Secondly, the predictions from classification must be understandable and trusted by the chemists within the pipeline. In this work, we study the trade-off between prediction accuracy and interpretability by implementing three document embedding methods that vary in computational complexity. With our accuracy results, we also introduce local interpretability model-agnostic explanations (LIME) of each prediction to provide a localized understanding of each prediction and to validate classifier decisions with our team of energetics experts. This study was carried out on a novel labeled energetics dataset created and validated by our team of energetics experts.

Behavior of ADN-prills in microfluidic emulsion crystallization process

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Keywords: ADN; crystallization; microfluidics.

Since ammonium dinitramide (ADN) is a future-oriented green oxidizer in solid rocket propellants and a promising candidate to replace the environmentally harmful ammonium perchlorate, the focus of the current research lies on propellant formulations with ADN. For its implementation in a rocket propellant matrix, a spherical shape of the crystal is required. To achieve good control of crystallization in favor of prill quality, it is necessary to understand the crystallization kinetics of ADN melt droplets. Parameters like droplet size, supercooling temperature and addition of surfactants and additives have an impact on the crystallization behavior. The technique of microfluidics, as a powerful tool to investigate these parameters individually, was applied in this work.

Evaluation of nitropyrazole based nitrate esters as melt-castable energetic materials

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Keywords: pyrazole; nitrate ester; melt-cast explosive; crystal structure; secondary explosive.

Novel melt-castable explosives with a melting point between 80 and 110 řC are still desired because of the high toxicity and rather low performance of TNT. Several melt castable explosives bearing a nitratomethyl moiety on the pyrazole scaffold are presented. The compounds were obtained via straightforward syntheses and intensively characterized e.g. by IR, multinuclear NMR, mass spectrometry, elemental analysis and DTA or DSC measurements. Crystal structures were obtained by low temperature single crystal X-ray diffraction. The sensitivities towards impact, friction and electrostatic discharge were determined according to BAM (Bundesamt für Materialforschung) standard methods. The energetic performance of the prepared nitrate ester compounds was predicted by the EXPLO5 computer code, using recalculated X-ray densities and heats of formation from CBS-4M calculations. Additionally, the compatibilities with various high explosives were evaluated.

Spectroscopic, structural and energetic properties of pentanitroaniline

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Keywords: energetic materials; polynitrobenzenes; X-ray diffraction; NMR spectroscopy.

Although pentanitroaniline (PNA) has been known for almost 100 years, in the meantime with optimized synthesis, but still not fully characterized. In this contribution, the crystal structure of PNA is reported for the first time without any adducts or solvents, allowing view of the crystal packing, as well as the exact positioning of the nitro groups relative to each other. In addition, based on the crystal structure, a Hirshfeld analysis was performed, which allows to display the distances and types of interactions of the outer atoms. The compound was also studied in detail by NMR, especially with respect to 13C and 14N, making this a challenge due to sensitivity in solution. Furthermore, the compound was fully characterized by IR spectroscopy and TGA, as well as the sensitivities were measured. Using the density obtained from X-ray crystallography, as well as the heat of formation calculated with the GAUSSIAN program package, the energetic parameters were calculated using EXPLO5 computer code. The performance data were compared to the commonly used RDX and oxidizer ammonium perchlorate, as well as the structurally similar triaminotrinitro (TATB) and pentanitro (PNB) benzene.

Comparison of 1-vinyl 5H-tetrazole and 1-allyl-5H-tetrazole as ligands in energetic transition metal complexes

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Keywords: energetic coordination compound; tetrazole; sensitivity; priming mixture.

Energetic Coordination Compounds (ECC's) are one approach to generate new materials for priming mixtures. The concept is to combine the three building blocks: (i) ligand, (ii) transition metal, and (iii) anion, acting as (i) fuel, (ii) glue, and (iii) oxidizer or energetic component. By variation of the ligands the complexes' properties can be adjusted toward their desired performance and sensitivities. In the present study, 1-vinyl-5H-tetrazole (1-VTZ) and 1-allyl-5H-tetrazole (1-AllylTZ) were used as nitrogen-rich endothermic ligands to form 3d metal based ECC's. The new ligand 1-VTZ was prepared by elimination of hydrogen chloride from 1-(2-chloroethyl)-5H-tetrazole in methanolic KOH solution, whereas 1-AllylTZ was obtained by a heterocyclization reaction of allylamine with triethyl orthoformate and sodium azide in acetic acid medium. All compounds were intensively characterized with analytical methods such as XRD, IR, EA, DTA, TGA and sensitivity measurements (IS, FS). The energetic performances were evaluated by hot needle, hot plate, and laser initiation experiments.

PBX compositions based on high explosives and polymeric binders with adjustable water solubility

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Keywords: energetic materials; polymers; binders; water soluble.

The harsher and increasingly complex international and European environmental legislation drive the effort for the development of greener energetics and munitions. In this context the aim of this paper is to present the continuation of our experimental study regarding PBXs based on high explosives (RDX) and novel acrylic acid/alkyl acrylate copolymeric binders. Their adjustable water solubility at various pH values allowed, in the previous study, the facile recovery of the explosive in its original shape and morphology. Based on the same binder system with adjustable water solubility, in this study we approached an eco-friendly coating technology for a simpler and safer manufacture, avoiding the use of consecrated organic solvents.

Differences between sample form and it's effect on sensitivity of composite propellants containing BCHMX as a new energetic additive

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Keywords: composite propellant; nitramine propellant; sensitivity.

This paper presents the results of friction and impact sensitivity of new energetic additive cis-1,3,4,6-tetranitrooctahydroimidazo-[4,5-d]imidazole (BCHMX) incorporated to composite propellant. Effect of concentration of energetic additive on friction and impact was studied. Results was compared to his structure analogue HMX and unmodified propellant. As samples, plates and powdered propellant was used in order to examine the differences between sample form and their response to mechanical stimuli. Different sensitivity values was obtained for each form of sample type. Effect of burning rate catalyst is also discussed. For evaluation of sensitivity FEST method was used.

Cylinder test of emulsion explosives: possibilities of detonation pressure estimation

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Keywords: emulsion explosives; cylinder test; JWL; detonation pressure.

Cylinder tests are widely used to characterize the behaviour of detonation products. The main output of the cylinder test is the equation of state (EOS) of the detonation products. The JWL EOS is frequently used because of its simplicity and its implementation in various hydrocodes. To describe the explosive for the purposes of JWL calculation, one needs to know its density, detonation velocity and detonation pressure. The measurement of detonation pressure is difficult, mainly for the cases of explosives with a long reaction zone. Four methods of detonation pressure estimation were therefore selected from the literature. The four resulting values of detonation pressure were taken as the input for the JWL calculation procedure, to obtain four sets of JWL parameters. Every set of the JWL parameters was used to simulate the wall motion during cylinder test using LS-DYNA hydrocode. All the simulated wall velocities are compared to the experimental ones for two samples of emulsion explosives. Based on this comparison, the usability of individual methods for the detonation pressure estimation is briefly discussed and evaluated.

Lithium 2,2,2-trinitroethyl nitrocarbamate monohydrate as colorant in red-burning pyrotechnics

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Keywords: nitrocarbamate; lithium salt; Lewis acid-base reaction; red pyrotechnic colorants.

Due to the negative effects of chlorinated components and strontium on human health and the environment in red-burning pyrotechnics, research into "green" substitutes has been increasing in recent years. One possibility to avoid the problems mentioned above, is the use of lithium. The use of lithium salts in strontium- and chlorine-free mixtures has already been investigated. Therefore, in this work we present the new lithium salt of 2,2,2-trinitroethyl nitrocarbamate. The synthesis is carried out starting from trinitroethanol, which was reacted with chloronylsulfonylisocyante (CSI) to give the corresponding carbamate. Subsequent nitration led to 2,2,2-trinitroethyl nitrocarbamate, followed by an acid-base reaction with lithium hydroxide to form the lithium salt. The new compound was extensively analyzed by IR, EA, DTA and multinuclear NMR (1H, 13C and 7Li) spectroscopy. Furthermore, the sensitivities towards impact and friction were determined according to BAM standards and the energetic performance was calculated using EXPLO5 code. The performance of the salt in pyrotechnical mixtures was evaluated in terms of dominant wavelength, light intensity, color purity and burning time.

Reduced sensitivity RDX and HMX crystallized and spheriodized in propylene carbonate

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Keywords: RDX; HMX; propylene carbonate; sensitivity; spherical.

Energetic materials were crystallized from propylene carbonate solutions with the help of fatty acids. From tested additives, stearic acid causes formation of more spherical and less defect crystal materials. Obtained reduced sensitivity RDX was less impact sensitive in comparison with starting material (7.5 J, 15 J resp.) and also less friction sensitive (110 N starting RDX, 160 N crystallized). HMX and RDX crystals were then spheriodized in propylene carbonate suspension at a constant temperature for 2-4 hours. Final spherical or oval-shaped crystal materials were submitted to GAP test and mechanical sensitivity tests.

Prediction of ANFO's charge diameter effect on detonation parameters using hydrodynamic and thermochemical codes

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Keywords: ANFO; thermochemcial code; hydrodynamic code.

ANFO explosive exhibits highly non-ideal behavior that is characterized, among other things, by the strong dependence of detonation velocity on explosive charge diameter. Such behavior cannot be modeled by the ideal detonation model and must include both rates of radial expansion of detonation products and the rate of chemical reactions in the detonation reaction zone. In this paper, we used hydrodynamic code AUTODYNE and thermochemical code EXPLO5 coupled with the Wood-Kirkwood detonation theory to predict the effect of charge diameter on detonation parameters of ANFO explosive. Both EXPLO5 and AUTODYNE are supplemented with a single-step pressure-based reaction rate model and equations of state of unreacted ANFO and detonation products. It was shown that both calculations can reasonably well reproduce experimental detonation velocity – charge diameter results provided the reaction rate model is calibrated properly.

Ballistic modification of extruded double base propellants

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Keywords: copper oxide; ballistic modifier; extruded double base propellants.

Copper(II) oxide is widely used as a burn-rate catalyst (or "ballistic modifier") in double-base propellant formulations, normally in conjunction with compounds of lead. The phenomenon of plateau-mesa burn rates – a pressure interval across which the burn rate remains essentially constant or declines slightly with increasing pressure – is thought to be largely induced by the lead-based ballistic modifiers, whereas copper(II) oxide induces a more general acceleration of burn rate across a wide pressure interval.

The particular properties of copper(II) which influence its catalytic performance ("ballistic activity") are unclear, and wide variations in the ballistic activity of different samples of copper(II) oxide have been observed, even in cases where the samples are almost identical in terms of purity, phase, surface area and porosity. All commercially-available grades of copper(II) oxide tested so far have exhibited poor ballistic activity, and so CEUK have conducted trials to identify process conditions which consistently produce ballistically active copper(II) oxide. One indicator of high ballistic activity in the past has been a mass loss of >2.5% on calcination of copper(II) oxide made by the titration of copper(II) nitrate with sodium hydroxide; this produces basic copper nitrates (BCN) as an intermediate species and the observed mass loss is a possible indicator of the presence of residual BCN in the copper(II) oxide. However, BCN was not detected by X-ray or by surface analyses of these samples, but it is possible that the particles of copper(II) oxide contain an amorphous kernel of this material.

CEUK have trialled two general synthesis routes; one in which intermediate BCN is isolated and dehydrated in an oven, and another where copper(II) oxide is formed directly in the reactor during titration of copper(II) nitrate via conditions of high temperature and pH. Material from the latter process has shown promising ballistic activity.

Oxetan-3-one as promising building block for energetic monomers

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Keywords: oxetan-3-one; Schiff base; energetic monomer; crystal structure; explosive.

New energetic monomers suitable for ring-opening polymerization and the corresponding polymers are more useful as binders than the currently in used non-energetic HTPB (hydroxyl-terminated polybutadiene). Well known energetic monomers based on oxetanes are 3,3-(bisazidomethyl)oxetanes (BAMO) or 3-(nitratomethyl)-3-(methyl)oxetanes (NIMMO) which are known since the 1970s. Meanwhile oxetanes such as oxetan-3-one have become commercially available because of their use in pharmaceuticals. In this work, we present a series of new energetic oxetane monomers based on oxetan-3-one and also spiro compounds which are suitable for cationic ring-opening polymerization. Oxetan-3-one is condensed with different compounds with hydrazines functionalities such as aminonitroguanidine (ANQ), picrylhydrazine (PicHy) and 1,5-diaminotetrazole (1,5-DAT) to get new monomers. Upon reaction of the oxetane-guanidine compounds with hydrazine, spiro compounds are formed leading to 1,2,4,5-tetrahydro-1,2,4,5-tetrazines. All products were extensively analyzed using IR, EA, DTA and multinuclear NMR (1H and 13C) spectroscopy. The crystal structures of the solid products were elucidated using single crystal X-ray diffraction. In addition, the sensitivities toward impact and friction were determined according to BAM standard and the energetic performances of the condensation products as well as the spiro-tetrahydrotetrazine compounds were calculated using the EXPLO5 code.

Tunable energetic materials from 4-nitro-1,2,3-triazole

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Keywords: energetic materials; heterocycle; primary explosive; triazole.

Previously known 1-amino-4-nitro-1,2,3-triazole and its isomer 2-amino-4-nitro-1,2,3-triazole were produced by N-amination of 4-nitro-triazole with O-tosylhydroxylamine. They were then azo-coupled to produce two new energetic materials WPX-101 and WPX-102. All compounds were fully characterized as energetic materials and were found to be primary explosives. These materials have differences in their sensitivities and performances that are attributed to their differences in connectivity, with WPX-101 possessing performances similar to that of HMX.

Comparison of plastic bonded enhanced blast explosive with TNT and Comp-B in terms of thermal and blast properties

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Keywords: enhanced blast explosives; pressure impulse; thermal impulse.

Enhanced blast explosives, contain reactive metal component, have several advantages over conventional explosives such as TNT and Comp-B. Pressure impulse and thermal impulse of enhanced blast explosives are higher than TNT or Comp-B, hence the destructive power is increased. Detonation of enhanced blast explosives also results in larger dimension of fireball and longer fireball duration. These advantages are provided with the heat generated by the combustion of metal powder in post detonation reaction. In this study, plastic bonded enhanced blast explosives that contain 30% (TSP-01-1) and 45% (TSP-01-2) by weight metallic aluminum powder were developed. Then, these developed explosives were analyzed with respect to thermal and blast effects through open and closed area performance tests. The results of these tests were compared with the same volume of conventional explosives and showed that the thermal and blast performance of TSP-01-1 and TSP-01-2 explosives were higher than TNT and Comp-B. Radiant intensity of flame and maximum diameter of fireball for TSP-01-1 and TSP-01-2 explosives were also higher. Pressure impulse values of TSP-01-1 and TSP-01-2 explosives were at least 30% higher than conventional explosives.

In search of new commercially available bonding agents for RDX/HTPB compositions

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Keywords: bonding agents; PBX; HTPB; RDX.

To determine effectiveness of different compounds with potential bonding activity, series of RDX/HTPB samples were prepared and tested. The samples consisted of bimodal RDX, HTPB with high content of 1,2-vinyl groups, isophorone diisocyanate (IPDI) as curative, bis(2-ethylhexyl) adipate (DOA) as plasticizer, dibutyltin dilaurate (DBTDL) as curing catalyst and several different compounds with potential bonding activity. Density, hardness and detonation properties (for selected samples) were determined. Polarized Light Microscopy was used to determine bonding activity of the chosen compounds. Samples containing hydantoin-based bonding agent were used as reference. As a result of the studies a new bonding agent was proposed, therefore further investigation must be conducted to its implementation in PBX formulations.

Keyword Index

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