Abstracts of the 23rd Seminar on

New Trends in Research of Energetic Materials

Pardubice, April 1–3, 2020

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Institute of Energetic Materials

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New Trends in Research of Energetic Materials

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Preface

This year's NTREM seminar takes place in the year of the centenary of the teaching of the science of explosives in Czechoslovakia, the centenary of the foundation of Explosia Co., Pardubice, and seventy years of the academic chemistry teaching in Pardubice.

The development of not only the production of explosives but also of corresponding science in the areas of the present-day Czech and Slovak Republics was preceded by several important events in Austria-Hungary already in the 18th century; in 1825 Mr. Sellier has founded in Prague a production of the percussion caps, from which soon evolved a well-known firm Sellier & Bellot for infantry ammunition. But main events were associated with Alfred Nobel. Under his direct supervision, the production of nitroglycerine was implemented and started in Prague-Zámky in 1868, making it the fifth in the world at that time. Subsequently, in 1873, Alfred Nobel initiated the production of dynamite and gun cotton near Bratislava (Dynamite Nobel) in present-day Slovakia. The company in Slovakia soon built a network of its plants in the Austrian-Hungarian monarchy and expanded abroad (for example, to the Transvaal province of South Africa in 1895) – the Dynamite Nobel Works acquired strategic importance as a major supplier of munitions for the land and naval forces of Austria-Hungary. These facts, together with the First World War, contributed to the education of domestic explosive specialists. After the establishment of Czechoslovakia in 1918, they engaged in the development of the respective production and in the introduction of the teaching specialization in the new state. In 1920, these scientific and educational activities were initiated at the Prague Institute of Chemical Technology (now the University of Chemistry and Chemical Technology, UCCT), led by Prof. Ing. Dr. Cyril Krauz. In the same year, a factory for explosive substances, Explosia, was established in Prague with production in Pardubice (the production from Bratislava and Prague-Zámky was moved there); this was another milestone in the development of the specialization. These two events significantly influenced the development of energetic materials in Czechoslovakia. Along with the high level of the Czech engineering industry at that time, this led to the fact that Czechoslovakia before the Second World War became a significant producer and exporter of weapons, ammunition and explosives with an appropriate scientific research and engineering base. Teaching activities were discontinued during the Second World War, i.e. in the 1939–1945 period, when Czech universities in the Czech lands, occupied by the Hitler's army, were closed. After the post-war renewal of scientific and educational activities at these schools, the sub-specialization 'Special Production Technology' was established at the UCCT in Prague in the academic year 1952/1953. Its management was entrusted to Dr. Ing. Josef Seifert, who (through his personal contacts in Pardubice) prepared the establishment of the Department of Special Productions (DSP) at the local Institute of Chemical Technology Pardubice (ICT) in the same academic year. This institute, a predecessor of the present-day University of Pardubice, was founded there in 1950. The predecessor of the current Institute of Energetic Materials (IEM), i.e. the DSP at the ICT in Pardubice, was officially established in September 1953. After the Second World War, Czechoslovakia never regained its former position in the export of weapons, ammunition and explosives. However, the export of these commodities became very significant for its economy again. Nevertheless, this importance was not reflected in the support of scientific and educational activities of the Department of Special Productions on the part of the management of the ICT Pardubice. This adversity resulted in the abolition of the department as a separate workplace as of 1966. The department was renewed in 1986 by the former long-term director of the Research Institute of Industrial Chemistry (RIIC) in Explosia, Assoc. Prof. Boris Vetlický, who had pushed this change through by the strength of his personality. However, the IEM was almost closed between 1994 and 1999 as a consequence of a severe staffing crisis, when also the Czech industry was in disintegration. In the last five years, there has been a successful effort to renew activities in the defense industry in the Czech and Slovak Republics. The IEM has also undergone significant positive development over the past ten years, mainly thanks to the activities of its staff. However, there is still a substantial barrier in cooperation with foreign colleagues, which cannot be overcome by the IEM itself without the involvement of the university's leadership (such as a license for trading military materials).

International NTREM seminars, organized by the IEM since 1999, have significantly contributed to the promotion of this Institute in the world and to its development. The organizational measures that were already applied to the 22nd NTREM Seminar (i.e. the review of lectures by the Scientific Committee and the introduction of registration fees) have made it much easier for the Organizing Committee to prepare this year's meeting. A great job concerning this new organization of the NTREM seminar has traditionally been done by our Organizing Committee under the leadership of Assoc. Prof. Jiří Pachman with members of this committee, especially the treasurer Dr. Marcela Jungová, the co-editor of the proceedings Dr. Šelešovský and the representative of the dean's office Dr. Iva Ulbrichová; many thanks are owed to them for their perfect organization and services.

The registration fee introduced the last year was aimed at the elimination of non-serious contributions on the one hand while not limiting the attendance of young participants on the other. As such, it was set to such an amount that is insufficient to cover the costs of the seminar, thus making it necessary to rely on traditional supporters. The seminar is sponsored by a number of institutions and individuals, which enables the attendance of a wide range of participants, including students and young researchers not yet well financially covered by research grants. The organization of the 23rd NTREM Seminar in 2020 was made possible thanks to the following supporters:

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- ZVS holding, a.s.

The efficient help in ensuring the smooth and successful course of the meeting received from all of these institutions as well as supporters from the Seminar participants is gratefully acknowledged.

What else should be added on the occasion of this 23rd NTREM Seminar? Traditionally, first of all, I would like to express the following wishes: May its proceedings be successful and may the Seminar bring inspiration and pieces of knowledge for use in further scientific-research activities in the area of energetic materials, may it enable the establishment of new contacts and the deepening of the existing ones particularly between young participants in this meeting, and may the participants feel at home throughout the Seminar. Finally, I thank the members of the Scientific Committee, the authors of all the submitted papers and, last but not least, you, the participants in this seminar, for its success and its influence on the continued prosperity and growth of all future meetings at our university of young people and university teachers working in the field of all kinds of energetic materials.

Pardubice, March 15th, 2020

Svatopluk Zeman

Computational strategy for improving detonation performance of energetic materials

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Keywords: detonation performance; solid-state energetic materials; computation and experimental verification; preferred physicochemical characteristics.

We perform high throughput quantum calculations for extensive energetic crystals on modern supercomputers and reveal the mechanism how physicochemical characteristics control the detonation performance of energetic materials. The detonation velocity, detonation pressure, heat of explosion and detonation temperature of the solid-state energetic materials have been calculated and thoroughly verified by experiments. We extract the preferred molecular backbones, functional groups, detonation products and crystal characteristics of high-performing compounds and provide the computational strategy for obtaining high-performing energetic crystals.

Thermal behavior of CL-20 under the effect of Multi- Walled Carbon Nanotubes - doped with complexes of Nickel-Polydopamine

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Keywords: graphene-doped complexes of polydopamine; molecular dynamic simulation.

The graphene - doped complex of Polydopamine (PDA) were prepared for using as a promising energetic catalyst for decomposition of hexahydro-1,3,5-trinitro1,3,5-s-triazine (RDX). The decomposition kinetic parameters and mechanisms of the complex have been studied by means of differential scanning calorimetry/thermogravimetric techniques and supported by theoretical evaluations using molecular dynamic simulations.

High pressure characterisation of 3,4,5-trinitropyrazole

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Keywords: high pressure neutron diffraction; energetic materials; trinitropyrazole.

Nitrazole-based energetic materials have attracted attention as promising alternatives to conventional energetic materials with their energetic performance and sensitivity. Pyrazole and its nitro-derivatives have a significant role in azole-based compounds and can be classified as green energetic materials, since they release a large amount of dinitrogen gas as a detonation product, which is neither toxic nor environmentally harmful. Highly nitrated pyrazoles are expexted to be powerful explosives as well as effective ingredients for rocket propellants. Oxygen balance, density, detonation velocity and thermal stability of these compounds can be enhanced by adding nitro groups to the pyrazole ring. 3,4,5-trinitropyrazole (TNP) has been highlighted for its high energetic content, good thermal and chemical stability and low sensitivities to impact, friction and spark [1,2,3].

Investigation of the thermomechanical and polymorphic behaviour of energetic materials under high-pressure/temperature conditions is essential, as they experience such conditions during initiation and detonation. Their energetic performance is highly dependent on the particular polymorph which forms at detonation conditions, such as high pressure and temperature [4]. Given the importance of trinitropyrazole as a promising explosive and propellant, it is important to explore its high-pressure behaviour, determine its equation of state (EOS), and identify any pressure-induced polymorphic phase transformation. In this study, high-pressure Raman spectroscopy and high pressure neutron powder diffraction experiments were conducted in order to observe structural changes of 3,4,5-trinitropyrazole with increasing pressure.

Thermo-chemical decomposition of RDX in cyclohexanone and gamma-butyrolactone

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Keywords: ARC; heat flow microcalorimetry; RDX in cyclohexanone; RDX in gamma-butyrolactone; kinetic evaluation.

To improve its crystalline quality, RDX is processed in suitable solvents, among them are cyclohexanone and gamma-butyrolactone. In spite of its relatively high thermal stability, RDX can decompose to a certain extend during processing. Several qualities of RDX were investigated: so-called insensitive RDX (I-RDX) from Eurenco, Sorgue, France and so-called sensitivity reduced RDX (S-RDX) from Chemring, Saetre, Norway. With ARC^{TM} (Accelerating Rate Calorimetry) solutions between 6 mass-% and 10 mass-% of RDX in the two solvents have been used with 1 inch titanium ARC^{TM} bombs. The used instrument was so-called ES-ARC from THT Inc. Bletchley, MK1 1SW, UK. It was operated in the so-called 'ĂŸheat-wait-search'ĂŹ mode to register the decomposition exotherm reached by pseudo-adiabatic selfheating. The temperature range of detected decomposition is between 130řC and 230řC. The amount of RDX was used-up during the course of the full decomposition curve, means after the end of selfheating all RDX was consumed. The curves show an initial faster increase in self-heat rate. Mostly this is indicative for chemical species, which accelerate decomposition. Such features can be caused autocatalytically or by impurities. The curves were described with reaction kinetic models and Arrhenius parameters have been obtained. The heat flow microcalorimetry (HFMC) measurements were performed with TAM^{TM} III and a modified TAM^{TM} II instruments from TA Instruments. Isothermal measurement temperatures were between 80řC and 130řC.The data evaluation was done by differential iso-conversional description. To have an indication about the amount of RDX decomposition in the HFMC runs the solution were analysed with HPLC to find out the residual RDX content in the solutions. The curve shapes of heat flow curve (dQ/dt) and integrated heat flow indicate self-accelerating decomposition.

Carbon materials action on the 1,1'-ferrocendicarboxylic acid salts efficiency on combustion of double-base propellant

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Keywords: double-base propellant; burning rate modifier; carbon materials; carbon nanotube; X-ray electron-probe microanalysis.

The effect carbon nanotubes (CNT) and carbon black on the burning rate of double-base propellant with 3% of copper and iron salts of 1,1'-ferrocendicarboxylic acid (CFDA and IFDA, respectively) was investigated. Burning rate modifier efficiency was evaluated by the parameter Z=Uc/U0, where Uc - burning rate of the propellant with the catalyst, U0 - burning rate of the base propellant. It was shown that CNT have the greatest effect on the modifiers efficiency. Thus, propellant with 3% CFDA at p = 2MPa has Z=1.9, addition of 1% CNT to the propellant with 3% CFDA increases Z value to 4.2, and 1% carbon black has no significant effect on the burning rate of propellant with catalyst (Z = 2.0). As opposed to CFDA, 3% IFDA does not change the burning rate of the propellant. Addition of 3% IFDA with 1% CNT considerably increases burning rate (Z = 2.5 at p = 2MPa). Using scanning electron microscopy and X-ray electron probe microanalysis, the structure and composition of the combustion surfaces of the propellant with modifiers added both individually and with CNT and carbon black were studied. It was found that a significant catalytic effect is observed only if a carbon frame forms on the combustion surface, on which significant accumulation of modifier particles occurs. A higher frame is formed on the combustion surface with the use of CNT, in comparison with carbon black. It covers almost the entire combustion surface, which explains the significant increase in the modifiers efficiency when used with CNT. In the presence of 3% IFDA the carbon frame is not formed on the propellant combustion surface. The structure of the modified sample is similar to the structure of the base propellant. Opposite to that sample, carbon frame with accumulated catalyst particles is observed on the surface of quenched propellant with 3% IFDA and 1%CNT. Exothermic reactions are undergoing on the carbon frame and since the heat conductivity of the carbon frame with substantive amount of metal is higher than the conductivity of the gaseous zone, then the heat flow to the condensed phase from the carbon frame zone significantly increases, which leads to increasing of burning rate of the propellant.

Thermal decomposition of nitropyrazoles: Interplay of predictive electronic structure theory and thermal analysis

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Keywords: pyrazoles; thermal decomposition; highly accurate quantum chemical calculations; DSC; calorimetry; thermal analysis; formal kinetics.

Nitrogen-rich heterocycles and their derivatives are promising environmental friendly energetic compounds. In the present work, we studied kinetics and mechanism of thermal decomposition of 3,4- and 3,5-dinitropyrazole (3,4-DNP and 3,5-DNP, respectively), as well as 5-amino-3,4-dinitropyrazole (5-ADP) using a complementary combination of thermal analysis and quantum chemical calculations. Differential scanning calorimetry (DSC) measurements accompanied by FTIR detection of gaseous products were performed at atmospheric and elevated pressures (up to 5 MPa) under different heating rates (0.1 - 20 K/min). The experimental data were processed using isoconversional and formal kinetic approaches. 3,4-DNP and 3,5-DNP exhibited significant evaporation overlapping with the decomposition kinetics. The increase of the external pressure renders the decomposition kinetics to be dominant. At the same time, the presence of amino group in the structure of 5-ADP significantly affects thermolysis, resulting in strong autocatalytic nature of the kinetics. Experimental kinetics was complemented by the highly accurate CCSD(T)-F12 quantum chemical calculations to justify the use of particular reaction models and make comparison with the kinetic parameters for the dominating primary thermolysis reactions. Among the reaction pathways, the radical reaction of C-NO2 bond scission, the intramolecular oxidation, hydrogen transfer, and nitro-nitrite rearrangement were considered. The most energetically favorable channels for 3,4-DNP and 3,5-DNP turned out to be the nitro-nitrite rearrangements with the activation barriers 56 kcal/mol and 62 kcal/mol correspondingly, while in the case of 5-ADP the H-transfer from amino to nitro group dominates (barrier 33 kcal/mol). The relationship between the thermal behavior and structure of the species will also be discussed to give a guidance for design of novel molecules with increased stability.

Modifying the ignition and combustion performance of the Al/KIO_4 system with the use of additives

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Keywords: thermite; ignition; additives.

Nanothermites have received a lot of attention due to the fact that they have the potential to perform better than their micron scale counterparts when comparing factors such as burn rate. They do however require different processing procedures in order to unlock this potential. This makes implementation of the systems into existing production lines difficult. The objective was to produce a micron-sized thermite formulation that approaches the performance of fast-burning nanothermites. This was achieved by addition of additives to the aluminium (Al) potassium periodate (KIO_4) system. Additives took the form of two additional aluminium fuelled thermites with either copper(II) oxide (CuO) or polytetrafluoroethylene (PTFE) as the oxidisers. The combustion performance and ignition sensitivity showed the greatest improvement for a composition consisting of [Al/KIO_4]:[Al/CuO]:[Al/PTFE] 90:10:5. This blend had an ignition temperature of 470 řC, and in confined burns its flame front propagation velocity approached 1 km/s. The ignition temperature is significantly lower than those reported for the base system when using nanoscale components, while the heat of reaction also showed a slight increase. The burn rate is especially impressive as these rates are traditionally only seen in systems utilising nanoscale components. The change in ignitability and combustion performance is most likely due to a change in the reaction mechanism. The Al/KIO_4 system reacts according to a gas-solid mechanism while the addition of the additives makes a condensed phase mechanism possible. This is due to the expected interaction between the first stage decomposition products of the potassium periodate and PTFE. The compounds formed in this interaction facilitate the removal of the protective oxide layer on the aluminium exposing the more reactive core.

Ethylenedinitramide as building block in energetic materials

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Keywords: ethylenedinitramine; energetic coordination compounds; structure elucidation; laser ignition; sensitivity measurements.

In order to develop new explosives (primary and secondary), the nearly forgotten high explosive etyhlenedinitramine was prepared in a cost-efficient manner by nitration and subsequent hydrolysis of 2-imidazolidone. The neutral compound was converted into several energetic salts (e.g. alkaline and guanidines) by simple acid base reaction. Also energetic coordination compounds were formed by the application of endothermic nitrogen-rich ligands and etyhlenedinitramide as the anion. The compounds were characterized by low temperature X ray diffraction, IR-Spectroscopy, elemental analysis and differential thermo analysis (DTA). The theoretical detonation performance was calculated by the EXPLO5 code. Sensitivity measurements were performed for every compound with focus on impact, ball drop impact, friction and electrostatic discharge. In addition, hot plate and hot needle tests were performed together with laser ignition experiments for several compounds.

Automated production of energetic materials using flow chemistry

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Keywords: synthesis; flow chemistry; TEGDN.

This paper describes the design and construction of a fully automated pilot plant using flow chemistry. Traditionally, most energetic materials, and other synthesised materials, have almost exclusively been prepared in batch reactors. This causes large risks, when large quantities of energetic materials are produced. Flow chemistry can significantly reduce the risks in many ways, such as improved temperature control and reduced amounts of energetic materials present at any place at the same time. Even though flow chemistry has many benefits, the technique is more complex to develop. The hazardous chemicals used in synthesis of energetic materials require pumps, piping, vents, reactors, regulators, purification modules etc. to be highly resistant. This will in some cases require development of suitable equipment for such a system. This paper will present an example of an automated system for flow chemistry production of energetic materials with triethyleneglycol dinitrate (TEGDN) as an example.

The effect of magnesium oxide as a stabilizer of nitrocellulose

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Keywords: nitrocellulose; spontaneous ignition; stabilizer; propellant; calorimetry.

Nitrocellulose (NC) is prone to spontaneous exothermic degradation even in room temperatures by a reaction with nitrogen oxides and nitric acid released from NC itself, which occasionally causes an accidental explosion during its storage process. In order to prevent such accidents, NC is mixed with aromatic compounds as a stabilizer like diphenylamine (DPA) and akardite II (AKII) that can trap nitrogen oxides into its aromatic ring. However, a problem has been raised; such conventional stabilizers show toxicity because of generating its nitroso-daughter products, which means the development of alternative stabilizers is highly demanded. According to the previous study, not only aromatic but also inorganic compounds showing alkaline in water such as magnesium oxide (MgO) reportedly functioned as a stabilizer. From this, we investigated the thermal decomposition behavior of NC containing MgO by measuring the heat and nitrogen-oxides release behaviors during isothermal conditions and evaluated the performance of MgO as a stabilizer of nitrocellulose.

Thermal characteristics of fluoropolymer coated boron powders

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Keywords: boron; fluoropolymer.

Boron is an attractive fuel additive for energetic material composites attributed to its high gravimetric (57.6 kJ/g) and volumetric combustion (111.3 kJ/cm3) enthalpies. However the practical applications of boron has been hindered by longer ignition delay and extended combustion times due to the presence of an oxide layer on the particle surface. The passivating boric oxide (B2O3), melts at 450 °C to form glassy layer and evaporates only above 1800 °C. The glassy oxide layer acts as a barrier for further diffusion of oxygen across the interface and inhibits the rate of boron oxidation. Among the numerous approaches that have been attempted to improve the ignition, coating of boron with a fluoropolymer is a prospective method. During the ignition, fluorine residues generated from the fluoropolymer will react with and remove the passivating layer as gaseous products, thereby reducing the ignition delay and promoting the oxidation of Boron. In this work, we investigate the thermo-kinetic behaviour of boron powders coated respectively with three commercial fluoropolymers; Viton, THV and PVDF. The coating percentage was limited to 4wt% to retain their particle nature. The oxidation behaviour of fluoropolymer coated boron was studied by thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). The kinetics of oxidation of the pristine as well as fluoropolymer coated boron was systematically studied by both Kissinger and model-free Kissinger–Akahira–Sunose (KAS) method. Heat of combustion was measured by calorimetry and the combustion residues were analyzed by powder X-ray diffraction. Kinetic analysis provided insights into the mechanism of oxidation of Boron as a function of the nature of the fluoropolymer used for coating. X-ray analysis of the combustion residues indicated that the extent of oxidation of boron has been promoted even by a thin layer of fluoropolymer coating.

Cocrystallisation studies of FOX-7 (DADNE)

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Keywords: FOX-7; DADNE; co-crystallisation; explosives; energetic materials.

The development of energetic materials (explosive and propellants) is currently focusing on co-crystallisation. This can enhance the performance of existing energetic materials by changing the physical and chemical properties of crystalline solids. This technique is also widely used and studied in the pharmaceutical sector, where properties such as dissolution rate, thermal stability and bioavailability can be modified without structural adaptation of the active pharmaceutical ingredient (API). In the past decade, there have been several reports about co-crystals of energetic materials, but interestingly there is only one about a co-crystal of 1,1-diamino-2,2-dinitroethene (FOX-7), a secondary explosive with low sensitivity to both impact and friction. This desirable property results from a combination of remarkable delocalisation occurring within the molecule and its extensive inter molecular and intramolecular hydrogen bonding. The preparation of co-crystals of FOX-7 can provide an opportunity to understanding of structure-property relationships in energetic materials. In this work, PPD (p-phenylenediamine) has been chosen because it would be possible to imitate the intermolecular interactions and interrupt the strong intermolecular hydrogen bonding of FOX-7 during co-crystallisation. A co-crystal of FOX-7 and has been successfully synthesised and structurally characterized by single-crystal X-ray diffraction, X-ray powder diffraction (XRD) and FTIR. The single-crystal study shows that the material crystallises in the monoclinic space group I2/a and the strong hydrogen-bonding present alters the conformation of the FOX-7 molecule. Sensitivity testing (BAM Fall Hammer) has been conducted and supports the idea that the new conformation affects the material's sensitivity.

Decomposition mechanism of o-nitrotoluene: New insights from predictive electronic structure theory

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Keywords: nitrotoluene; thermolysis; mechanism; quantum chemistry; explicitly correlated methods; multireference methods.

o-Nitrotoluene (NT) is a simple prototypical energetic material. A methyl group in the alpha position to a nitro group renders it an important congender of trinitrotoluene. Even though thermal decomposition of NT has been studied both experimentally and theoretically for more than a century, the mechanism of NT primary decomposition reactions still remains unclear. In the present work, we reexamined the gas-phase thermolysis of NT using an up-to-date predictive electronic structure methodology. The relevant points on the potential energy surface (PES) of NT were studied at the CCSD(T)-F12/VQZ-F12 level of theory. The CASPT2 geometry optimizations were employed in the PES regions with remarkable multireference character. The calculations revealed that the thermolysis of NT involves an intricate interplay of several closely lying decomposition channels and a number of transient species. More specifically, we identified an entirely new unimolecular channel leading to the most stable isomer of NT, viz., anthranilic acid. Apart from this, on the basis of computational estimations we declined a previously proposed water elimination molecular channel. Instead of this, the sequential radical elimination of OH and H closely competes with the anthranilic acid formation in the low-temperature thermolysis of NT. We also calculated the rate constant of C-NO2 bond scission, which is the dominant reaction in the high-temperature regime of NT thermolysis. To this end, we used the flexible transition state theory (FTST). In the framework of FTST calculations, the machine learning was employed for reliable and feasible construction of CASPT2 mutireference regions of PES pertinent to C-NO2 bond scission. The theoretically predicted rate constant of the radical reaction agrees with the most reliable experimental kinetic data up to a factor of 3.

Recent developments in the research of oxygen-rich energetic molecules

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Keywords: nitrate; trinitroethyl; X-ray; HEDO.

Several new compounds with high-oxygen content were synthesized from the divalent organic acids iminodiacetic and malonic acid. In this context, salts were compared to covalent compounds as well as perchlorate-free compounds with those carrying the more undesired perchlorate anion. The materials were readily available from the relatively cheap starting materials in straightforward synthesis. All compounds were characterized thoroughly by spectroscopic methods and crystal structures were determined through X-ray diffraction. In the further development, the thermal stability, the sensitivities against impact and friction as well as the densities were determined. For some promising new compounds, further physicochemical data were evaluated. Toxicological considerations have also been taking into account. The EXPLO5 V6.03 computer code was used to evaluate the performance parameters of potential energetic compounds in combination with CBS-4M calculated heats of formation.

The new energetic material bis(1-oxidotetrazol-5-yl)triazene and its corresponding C2N11O23- triple anion

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Keywords: tetrazoles; N-oxides; triazene; energetic properties; diazotation.

The structure of secondary explosives is mostly based on one of three motives: nitrated carbon frameworks (e.g. TNT), increased nitrogen content (e.g. RDX/HMX, TKX-50) or large cage- or ring-strain (e.g. CL-20). While the introduction of strains generally involves extensive laborious syntheses, the introduction of N-N single and double bonds can easily be realized, especially by azole chemistry. This work focuses on new energetic N-oxidized tetrazoles with a high nitrogen content. The well-known 1-hydroxy-5-aminotetrazole (5-ATO) was used as precursor to connect two 1-hydroxytetrazole units via a triazene linker in bis(1-oxidotetrazol-5-yl)triazene. The neutral compound as well as several salts were extensively characterized by low temperature single crystal diffraction experiments supplemented by NMR, EA, DTA and IR. The energetic performance parameters of all compounds were calculated using the EXPLO5 V6.05.02 program package. The calculated detonation velocities show a strong correlation between the weight of the cation as well as the amount of protons within the structure.

Detonation parameters of tetraamminecopper(II) nitrate (TACN)

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Keywords: cylinder test; detonation velocity; Gurney velocity; detonation pressure; impedance window; PDV; EXPLO5.

The tetraammoniumcopper complexes can be found as dangerous impurities in industry and also as easily available improvised explosives. This paper focuses on determination of detonation parameters of tetraammoniumcopper nitrate (TACN). Two cylinder expansion tests were performed using powdered TACN to determine Gurney velocity and JWL parameters of the detonation products. The particle velocity profiles were obtained using impedance window technique at the end faces of the charges and the detonation pressure value was estimated. For comparison, ideal values of the detonation parameters were also calculated using the EXPLO5 thermochemical code for TACN at the experimental density and at the theoretical maximum density.

Synthesis, isolation and characterisation of oligomer acetone peroxides

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Keywords: TATP; explosives; sensitivity; security; terrorism.

This presentation describes the characterisation of oligomers of acetone peroxide found as by-products during the production of triacetone triperoxide (TATP). The current study has been performed in the frame of the development of explosive standards used by European Commission and Member States' aviation security inspectors to verify the detection performance of explosive trace detection (ETD) in airports. Due to the importance of detecting TATP the JRC has developed an innovative spray (JRC-S4S-211) that can be safely used in public locations. The test spray enables security practitioners to verify the detection capabilities of explosives detection dogs and of ETD equipment. For production of a good quality standard, all impurities need to be properly characterised and quantified. Therefore efforts have been made to assess the purity of the produced TATP for optimal use in the test settings applying both to instrumental and canine detection. In this work, larger cyclic acetone peroxides like tetramer have been observed after HPLC/DAD analysis. The amount of these compound was directly linked to reaction time and the amount of catalyst used in the reaction mixture. The effect of acetone/hydrogen peroxide ratio to the yield of tetramer and larger cyclic peroxides were studied. An experimental design software was used to optimise the synthesis. The explosive properties like friction, impact, electric discharge and thermal sensitivity will be studied in the near future and compared to the more studied trimer and dimer, TATP and DADP.

Explosive derivatives of erythritol tetranitrate

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Keywords: ETN; derivatives.

Understanding the factors that affect explosive sensitivity is vital for the development of new higher performing and safer explosives. Studies have shown that sensitivity is influenced by fundamental chemical properties such as types of energetic functional groups and bond dissociation energies, as well as macroscale effects such as crystal packing and hydrogen bonding. Explosive functional groups can have differing stabilities due to differences in bond energies and decomposition pathways. While studies have been conducted on explosives with different functional groups, few involve systematic changes in these groups in order to alter the sensitivity of explosives. Erythritol tetranitrate (ETN) is an explosive that recently has attracted a lot of attention in the explosives community due to its ease of synthesis and good explosive characteristics. Herein we report the synthesis of ETN derivatives with azides and nitramines in order to test how functionalization of erythritol can alter explosive properties and sensitivities. Fully functionalized and mixed derivatives of ETN were prepared and tested for sensitivity and explosive properties. Mixing explosive functional groups led to changes in explosive sensitivity, explosive performance as well as physical properties including melting point and physical state at room temperature. Herein we have demonstrated that combining different explosive functional groups we can tune the explosive and physical properties of a molecule.

Deceleration of projectiles by liquid foam

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Keywords: liquid foam; Taylor gun; projectile; ballistics.

The detonation of improvised explosive devices (IEDs) generates significant lethality perimeters due to the propagation of shockwave and the ejection of projectiles. These risk areas can be reduced by shielding the explosive from the rest of the environment with a volume of liquid foam. Despite attenuating effects and apparent simplicity of use, the mechanisms for dissipating a blast wave and the deceleration of a projectile by these media are still poorly understood. In this study, we investigate the deceleration of a projectile by aqueous foam with controlled properties. Lab scale experiments are performed with neodymium spheres 1 cm wide, propelled by a Taylor gun and can reach 200 m/s. The magnets evolve in a PMMA pipe (50cm long and 6cm square section) filled with aqueous foam. Four round coils, 10cm wide are distributed every 15cm along the pipe. The measured voltage at the coil terminals is a function of the velocity of the projectile, according to magnetic induction arguments. Thereby, this device provides the velocity of the projectile inside the foam, despite the opacity of the medium. Two test programs are presented. The first one does not requires aqueous foam. The projectile is tracked using high speed cameras. Then the velocity of the projectile is correlated with signals obtained at the coil terminals. Finally, the accuracy and robustness of the method is evaluated. In the second test program, the pipe is filled with aqueous foam whose physical properties are controlled. The velocity of the projectile is measured upstream and downstream of the pipe with high speed cameras. The coils measure the velocity of the projectile inside the volume of foam. These experimental results are then compared to an analytical formulation of the drag force of the projectile in the liquid foam. Thereafter the mechanisms of dissipation of fragment energy by this type of medium are evaluated. Finally, the case of a supersonic projectile is discussed.

High-enthalpy organic components as dispersants of solid fuel for aircrafts with ramjet engine

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Keywords: solid fuel; ramjet engine; dispersant; high-enthalpy nitrogen-containing compounds; diethynylbenzene; flight range.

It was shown that it is possible to significantly increase the flight range of aircraft with a ramjet engine if, instead of ammonium perchlorate, organic high-enthalpy (more than 2 MJ/kg) compounds with a lower nitrogen and oxygen content relative to most explosives can be used as dispersants of solid fuel. The effectiveness of three-component fuels containing a hydrocarbon binder, boron and 50 different dispersants have been evaluated by the criterion of the flight range of the aircraft taking into account the completeness of fuel combustion in the afterburner. The most effective dispersants are recommended for further study. Among them there a few N-heterocycles such as 4H,8H-bis(furazano)-(3,4-b:3',4'-e)pyrazine; 7H-tris([1,2,5]oxadiazole)[3,4-b:3',4'-d:3",4"-f]-azepin-1-oxide; oxepino[2,3-c:4,5-c':6,7-c"]tris([1,2,5]oxadiazole) with the enthalpy of formation 2-3 MJ/kg and the α value (α=O/(2C+0.5H)) 0.25-0.50. This kind of dispersants can increase the flight range in 16-18%. If 1,4-diethynylbenzene is a dispersant the flight range increases in 1.7-1.8 times.

3D characterisation of ammonium nitrate powders by X-ray computed tomography

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Keywords: ammonium nitrate; prill; non-destructive characterisation; porosity; specific surface area.

The mixture of ammonium nitrate (AN) prills and fuel oil (FO), usually called ANFO, is extensively used in the mining industry as a bulk industrial explosive. One of the major performance predictors of ANFO mixtures is the fuel oil retention, which is itself governed by the porosity of the AN prills. Standardised tests routinely used to assess oil retention face several important limitations; the first being the difficulty to cover the wide range of porosity contents and morphologies from different types of ammonium nitrate prills; the second being the inability to evaluate the closed porosity, which is an important factor regarding the sensitivity of the explosive to detonation. In this study, we present how X-ray computed tomography (XCT), and the associated advanced data processing workflow, can be used to fully characterise the structure and morphology of AN prills. We show that structural parameters such as volume fraction of the different phases and morphological parameters such as specific surface area and shape factor can be reliably extracted from the XCT data, and that there is a good agreement with the measured oil retention values. XCT can therefore be employed to non-destructively and accurately evaluate and characterise porosity in ammonium nitrate prills.

TNT equivalence theory, solutions and problems

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Keywords: TNT equivalence; TNT equivalent; detonics; detonation; Gurney velocity.

TNT Equivalence has long been considered a known fixed quantity for an explosive. Many books, references and indeed Safety Regulations use the value for a particular explosive for safe Storage, Transport and Processing. This includes items like Quantity Distance (QD) for magazine storage of explosives. Unfortunately TNT Equivalence is actually an elusive number that depends on many things like ideal or non-ideal detonation, secondary combustion and the detonation parameter that is of your particular interest. So that the TNT Equivalence for an explosive differs for Blast Damage to that of Case Fragmentation. Casings also have a large effect on Equivalence, such that Ductile cases have radically different effects when compared with Brittle casings of the same mass, this also depends of the explosive. This paper will address these problems, theoretically address the issues and conclude with the outstanding problems identified.

Controllable Combustion Characteristics of Solid Propellants by Interactions of Al@PDA@Oxidizers

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Keywords: interfacial control; PDA; propellant; pressure exponent; agglomeration.

Solid propellants have received important applications in both military and civilization fields in the past century, where understanding the energy release mechanism and controlling the combustion process are the key issues to design and develop advanced propulsion systems. In this paper, core-shell structured Al@PDA@RDX and Al@PDA@AP micro-spheres with fine interfacial control have been fabricated by spray-drying technique, where poly-dopamine (PDA) is employed as a binding layer. These micro-spheres have been applied in HPTB-based composite propellants, which have the same theoretical formulation and hence identical specific impulse). However, these propellants differ in interfacial structure due to different ways of assembling the ingredients, resulting in significant changes in combustion performances. The thermal reactivity, burning rate, flame structure and condensed combustion products (CCPs) morphology of these propellants have been comprehensively investigated by the cutting-edge diagnosis techniques. It has been shown that the burning rate under low pressure could be improved by fine interfacial control of Al/Oxidizers, with increased flame temperature. Besides, these core-shell structured micro-spheres can greatly inhibit the large-sized agglomeration during combustion process.

Kinetics and mechanism of primary thermolysis reactions of bicyclooctogen (BCHMX) from highly accurate quantum chemical calculations

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Keywords: BCHMX; quantum chemistry calculation; thermal decomposition; kinetics gas-phase reactions; primary decomposition channels.

Cis-1,3,4,6-tetranitrooctahydroimidazo [4,5-d] imidazole (BCHMX) is a promising novel energetic component of solid propellants and plastic bonded explosives. Even though the thermolysis of BCHMX in the solid state and solution has been actively studied using both experimental and theoretical tools, its decomposition mechanism remains unclear. In the present work, we studied the primary gas-phase reactions of BCHMX thermolysis using the highly accurate and reliable DLPNO-CCSD(T) quantum chemical methodology. We considered a full set of 12 gas-phase conformers of BCHMX and identified those never discussed before. For all conformers we considered the radical decomposition (viz., N-NO2 bond scission) and a number of molecular channels, such as HONO elimination and several other isomerization reactions. Among the studied channels, the dominant role belongs to the radical decomposition with a N-NO2 bond energy of 41 kcal/mol. The activation barriers of other molecular channels turned out to be higher than 50 kcal/mol.

Detonation properties of the mixture of nitromethane/polymethylmethacrylate

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Keywords: detonation; liquid high explosive; nitromethane; polymethylmethacrylate; reaction zone structure.

Nitromethane is a typical liquid high explosive (HE), the detonation properties of which are determined by a chemical reaction occurring uniformly throughout the volume of the shock-compressed substance. The addition of various fine inclusions dramatically changes its shock-wave sensitivity and critical diameter [1-2]. This is a consequence of the appearance of hot spots in which the rate of chemical reaction increases and the decomposition of HE becomes inhomogeneous in the volume. Stabilization in time of the structure of the explosive mixture with glass microballoons is provided by increasing the viscosity of nitromethane by dissolving in it polymethylmethacrylate (PMMA) [1]. In this work, the structure of the steady-state detonation waves, detonation parameters and the dependence of detonation velocity on the amount of polymethylmethacrylate (PMMA) for the mixture of nitromethane/PMMA were investigated by a VISAR laser interferometer. It was found that at addition of 2 wt % PMMA and less the structure of particle velocity profiles and detonation parameters are very close to the neat nitromethane. At further increasing PMMA amount the detonation parameters begin to decrease and detonation front becomes unstable. When 4 wt % PMMA is added to nitromethane, the detonation velocity decreases from 6.30 to 6.21 km/s.

Time resolved pyrometry for deflagration

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Keywords: optical spectroscopy; pyrometry; HMX; deflagration.

Time-dependent visible light emission from energetic deflagration reactions has been studied. The shape of the greybody emission present allows the temperature of reaction to be measured, however spectral peak deviations may also be present in the optical emission. The construction of a three/four channel pyrometer is described that has wavelength channels chosen to avoid such spectral contributions, and allows a more reliable measure of the temperature evolution throughout reaction. The wavelengths are selected on the specifics of the reaction regime; in fall-hammer induced HMX deflagration, using the 400 to 500 nm region of band of wavelengths resulted in measured temperatures of 4000 ś 300 K. Although the intensity varied continuously thought the experiments, the measured temperatures were approximately constant throughout; indicating that the variation derives from changes in the instantaneous size of the emitting volume, rather than changes in reaction chemistry.

In Vitro Metabolism of TATP

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Keywords: TATP metabolism; analysis.

In the last decade terrorists have begun to use the homemade explosive triacetone triperoxide (TATP). As a result, law enforcement agencies and researchers needed to characterize it. Bomb detection dogs needed to be trained on it. This paper reports in vitro studies of its metabolism as a start toward the answer of its physiological effects and the potential of new forensic evidence.

Effect of TNT contaminated soil on vegetation in a controlled environment using UPLC-qTOF MS and FTIR profiling methods

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Keywords: TNT; metabolites; FTIR; UPLC-qTOF.

Two trees species (Freylinia lanceolate and Millettia Sutherlandii) and a grass (Eradrostis Superba) were each potted in 20 litre pots in order to evaluate the effect of 1,3,5 trinitrotoluene (TNT)-contaminated soil on vegetation. TNT contamination was established by dissolving flake TNT in acetone at 300 and 600 mg per kilogram soil concentrations. One pot for every species was left uncontaminated as control elements. A set of 9 samples, four contaminated, four uncontaminated aerial parts were gathered. These were processed and subjected to solid phase extraction method to isolate analytes of interests. Two laboratory analytical method were applied one that relies on Ultra-Performance Liquid Chromatography coupled to quadrupole time-of-flight mass spectrometry (UPLC-qTOF MS) and the other on Fourier-Transform Infrared Spectroscopy (FT-IR). For the UPLC-qTOF MS a gradient for the mobile phase was found which allowed the profiling and separation of metabolites in the aerial parts of the vegetation. These methods allowed identification and quantification of major changes caused by TNT contaminated soil on vegetation. The Synapt High Definition Mass Spectrometer SYNAPT HDMS G1 was operated using the electrospray ionization (ESI) technique in both positive and negative mode. A clear comparison for both UPLC-qTOF MS profiles as well as by FT-IR was achieved and has proven uptake of TNT residues by the plants.

Investigation on energetic coordination compounds with ammonia

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Keywords: explosives; coordination compound; explosive complex; ammonia complex.

Coordination complexes form a significant group of energetic materials. They are mainly considered as novel primary explosives. In this work we present the results of our research on explosive complexes containing ammonia as a ligand. These materials have been tested using various analytical techniques: elemental analysis, infrared spectroscopy, differential thermal analysis, and thermogravimetry. Sensitivity to mechanical stimuli was tested according to BAM standards. Moreover, to assess explosive properties, some of the test methods, such as measurements of critical diameter, velocity of detonation, blast wave parameters, heat of detonation and brisance, were carried out.

Copper complex of 5,6-bis(ethyl-nitroamino)-N'2,N'3-dihydroxypyrazine-2,3-bis-(carboximidamide): synthesis, characterization and ignition studies

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Keywords: laser ignitable materials; energetic copper complexes.

Development of new energetic compounds and formulations, suitable for ignition with relatively low power lasers, is a highly active and competitive field of research. The main goal of this effort is focused on achieving and providing much safer solutions for various detonators and initiators systems. In the present work, we prepared, characterized and studied thermal and ignition properties of a new laser-ignitable energetic compound, based on 5,6-bis(ethylnitroamino)-N'2,N'3-dihydroxypyrazine-2,3-bis(carboximidamide) (DS3) ligand. This new ligand was prepared in three steps, starting with 5,6-bis(ethylamino)-pyrazine-2,3-dicarbo-nitrile and crystallography studies of its Cu(II) complex (DS4) revealed an "antenna-type" structure of the latter complex. DS4 exhibited on set decomposition temperature of 150 °C and was calculated to have velocity of detonation of 6.36 km·s-1 and detonation pressure of 15.21 GPa. Notably and in contrast to many other laser-ignitable materials, DS4 showed properties of a secondary explosive, having sensitivity to impact of 8 J, sensitivity to friction of 360 N and sensitivity to electrostatic discharge of 12 mJ. In laser ignition studies (diode laser, 915 nm), we found that a single pulse, with time duration of 1 ms and with total energy of 4.6 mJ, was sufficient for achieving a consistent and full ignition of DS4. Analysis of dual pulse experiments, with variable time intervals between the pulses, in addition to fast camera filmed laser ignition experiments unambiguously showed that DS4 undergo ignition via a photothermal mechanism. Our results suggest that this energetic copper complex DS4 has a significant potential for its future development to higher TRLs and for further integration into small-size safe detonation systems.

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.

Investigating interactions between nitroglycerin and various ballistic modifiers in rocket propellants

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Keywords: nitroglycerin; Pb ballistics; DFT; adsorption.

Ballistic modifiers are additives in double base propellants, comprised of nitrocellulose and nitroglycerin mixtures, where they are attributed to reducing the sensitivity of the propellant to temperature. In particular, lead-based modifiers generate plateau burning characteristics within a specified pressure-range, producing a steady fuel burn rate. However, European legislation seeks to restrict the use of lead in propellants due to land and wildlife contamination, and to minimise health risks to personnel handling and operating propellants. As the catalytic behaviour of lead-based additives within the propellant system is poorly understood, and attempts to simply replace the lead with other materials has met with limited success, there is now a need for a fundamental investigation into the effects of lead-based compounds on the chemical reactivity of double base rocket propellants. This research thus aims to investigate the interaction between nitroglycerin and various lead-based surfaces (Pb, PbO, PbO_2), which represent lead-based clusters that are thought to form on combustion. In this way we look to establish whether they can provide catalytically active surfaces for the binding of nitroglycerin compared to other metal oxides (SnO_2, Bi_2O_3, CuO), which in contrast show only modest catalytic function as a ballistic modifier. The most stable surface of each system was deduced, to which a nitroglycerin molecule was attached in a binding study. The optimised structures have been extensively analysed, with outcomes focusing on adsorption energies, electronic properties and changes in vibrational modes of nitroglycerin to identify bond weakening. This work has made use of the ab initio CRYSTAL17 code, with the range separated hybrid HSE06 functional and localised basis sets utilised alongside the Grimme D3 dispersion correction scheme.

Novel carbon nanomaterials coated with CuO particles via electroless plating for nonothermite applications

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Keywords: electroless plating; copper oxide coated carbon nanomaterials; carbon nanotube; carbon nanofibers; superthermites.

Carbon nanotubes (CNTs) and carbon nanofibers (CNFs) can be utilized for the preparation of superthermite particles. This study is focused on the synthesis and characterization of copper oxide (CuO) coated CNTs and CNFs via electroless plating. This technique offers uniform metallization for the distributed copper layer through annealing process at 250 řC. A coating of uniform copper oxide layer was described using TEM. Examining the developed hybrid carbon nanomaterials (CNMs) by XRD diffractograms revealed a highly crystalline CuO particles superimposed on the surface of CNMs. Furthermore, the CuO coating can act as an effective oxidizer for aluminium particles in superthermite applications. The CuO-coated CNMs were effectively dispersed in isopropyl alcohol with aluminium particles (100 nm) using ultra sonic probe homogenizer to form a nanothermite material. The resulted nanothermite material was carefully introduced to molten trinitrotoluene (TNT) intending to enhance its brisance. Kast test results declared an increase in the shock wave strength by 6.5 % for CuO-coated CNFs/Al binary mixture whereas 15.5% for CuO-coated CNTS/Al binary mixture. The superb performance of CuO-coated CNTs was ascribed to the extensive interfacial surface area of 700 m2/g consequently it could act as an ideal carrier for highly energetic particles.

The hydrolytic action of nitramino oxadiazole-based compounds

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Keywords: hydrolytic reaction; nitramino compounds; oxadiazole-based compounds.

Nitramino oxadiazole-based compounds are widely recognized as high-energy-density materials, such as [5,5'-dinitramino-2,2'-bi(1,3,4-oxadiazole)] (ICM-101), [5,5'-dinitramino-3,3'- bi(1,2,4-oxadiazole)] and so on. Their strong hydrogen bonds provided by nitramino group make these molecular remain almost planar structure and obtain high energy density. However, in our recently study, the oxadiazole-based compounds containing nitramino group are unstable in hot water. ICM-101 and [5,5'-dinitramino-3,3'-bi(1,2,4-oxadiazole)] will occur hydrolytic reaction when treated with boiling water and generate corresponding ketone form products. We successfully synthesized the hydrolyzed products of ICM-101 and [5,5'-dinitramino-3,3'- bi(1,2,4-oxadiazole)] via the hydrolysis process, and obtained the single crystal structures of their corresponding potassium salts and themselves. The crystal structure of hydrolytic product of ICM-101 is monoclinic, and its density is 1.908 g/cm3 at room temperature, and the crystal structure of its potassium salts contains four H2O, so the density is only 1.813 g/cm3. This will provide experimental supporting information for us to understand the properties of nitramino oxadiazole-based compounds and the unstable factors in their synthesis procedure.

Photocatalytic processes in laser initiation of energetic materials

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Keywords: laser initiation; photocatalysis; spectroscopy; metal oxide.

Laser initiation of high energy density materials provides exciting new opportunities in fundamental science and applied technology for various applications, especially if it is about improving the safety of high explosive materials and devices. The development of energetic materials resistant to shock and heat but sensitive to laser radiation is the main goal of this research area. Considering the laser initiation process from the photochemical point of view can help to achieve this goal. Approaches of the energetic materials sensitization to laser radiation by introducing metal oxides as a photocatalytic additive were proposed and discussed in this report. Laser radiation dramatically decreases the decomposition reaction potential barriers of the energetic material included in the organic-inorganic interface with wide-gap metal oxides. Photoinduced charge transfer was proposed as a process driver. Two types of photocatalysts with different charge transfer paths were tested. UV-VIS-NIR spectroscopy and laser initiation test results concurring with DFT calculations were reported.

Studies of the detonation ability of the hydrazine salt of 5-aminotetrazole

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Keywords: hydrazine salt of 5-aminotetrazole; detonation ability; velocity of detonation; bkw equation of state.

The detonation ability of hydrazine salt of 5-aminotetrazole (HAT) has been experimentally studied. In a charge with a diameter of 28 mm (with a density of 0.8 g/cm3) in a thick-walled steel shell it is not possible to cause detonation even when using an intermediate detonator in the form of 10 g explosion cartridge of RDX. The study of mixtures of HAT with PETN showed that the experimental velocity of detonation is much lower than that calculated by the thermodynamic method. For example, for a mixture of 80% HAT 20% PETN, the measured velocity of detonation at a charge density of 0.8 g/cm3 is 4 km/s, while the calculated value is more than 1 km/s higher. An analysis of the probable causes of the discrepancy between the calculated and experimental values of the velocity of detonation is discussed.

Optimization of aluminized HMX-based explosive mixture

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Keywords: optimization; RSM; aluminium; HMX; explosive mixture.

The optimization of HMX-based explosive mixtures was studied in this paper. Explosive mixtures primarily consist of HMX and HTPB as a binder. In order to obtain explosive mixtures with higher energy output different amounts of aluminium and ammonium perchlorate has been used in the explosive mixtures. Response surface methodology (RSM) experimental mixture design is used on quantitative data from the experiment to determine regression model and to statistically optimize output variables. The output variables are detonation velocity and heat of detonation. The explosive mixture is optimized using reduced number of experiments and giving statistically significant desirability of 0.887.

Simulations of benzotrifuroxan and hexanitrobenzene cocrystal (1 :1) structure

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Keywords: atom-atom potentials; molecular electrostatic potential; force fields; crystal structure prediction; sublimation enthalpy; enthalpy of formation; molecular crystal density; detonation characteristics.

Based on the previously developed methodology of optimized distributed charges approximating the molecular electrostatic potential and using the original computer program for grid-scanning of potential energy surface, the simulation of benzo[1,2-c:3,4-c':5,6-c"]tris[1,2,5]oxadiazole, 1,4,7-trioxide (BTF) and 1,2,3,4,5,6-Hexanitrobenzene (HNB) crystal structures with the different sets of Atom-Atom Potentials (ECEPP, ECEPP-05, FIT, Williams 01, Combes 1996) was established. Effective AAP-s sets were determined, the use of which allows us to model the structure of the crystal lattices closest to the X-ray structural experiment. On the base of these sets the simulation of the most energetically favorable structure of BTF and HNB (1 : 1) co-crystal was carried out. The molecular crystal density, the enthalpies of sublimation and formation for individual BTF and HNB and their co-crystal were calculated as well as some detonation characteristics.

Combining performance with thermal stability: Synthesis and characterization of 5-(3,5-dinitro-1H-pyrazol-4-yl)-1H-tetrazole and its energetic derivatives

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Keywords: energetic materials; polynitro azoles; high explosives; energetic derivatves.

The demand for better, more efficient and environmentally friendly high-energy dense materials (HEDMs) in the military but also in the civilian sector is constantly increasing. Nitrogen-rich heterocycles play an important role as building blocks in the development of new energetic materials. During the past decades, various different five- and six-membered heterocycles (e.g. pyrazoles, triazoles, tetrazoles, tetrazines) were investigated extensively with regard to their suitability as potential new high explosives. 3,3ť5,5ť-Tetranitro-4,4ť-bipyrazole, bis(3,4,5 trinitro-pyrazol-1-yl)-methane and dihydroxylammonium 5,5ť-bitetrazole-1,1ť-dioxide are substantial examples for azole based explosives which exhibit not only good stability toward external stimuli but also show high performance. In this study we present the synthesis of 5-(3,5-dinitro-1H-pyrazol-4-yl)-1H-tetrazole and its energetic derivatives starting from 4-amino-3,5-dinitropyrazole, which was diazotized and cyanide substituted. A subsequent cycloaddition reaction with sodium azide led to 5-(3,5-dinitro-1H-pyrazol-4-yl)-1H-tetrazole (1). Several alkali metal and nitrogen-rich salts (ammonium, hydrazinium, guanidinium, aminoguanidinium and hydroxylammonium) were prepared and characterized by low-temperature X-ray diffraction. Additionally, all compounds were analyzed by vibrational spectroscopy (IR) 1H and 13C NMR spectroscopy, elemental analyses and differential thermal analysis (DTA). Additionally the heats of formation for anhydrous compounds were calculated using the atomization method based on CBS-4M enthalpies as well as some detonation parameters by using the EXPLO5 code (V6.05). Furthermore, the sensitivities of 1 and selected salts toward friction, impact and electrostatic discharge were determined.

Influence of distance from detonator on detonation velocity for different double base propellants

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Keywords: detonation velocity; propellant.

Steady-state detonation is characterized by constant values of detonation parameters. In such conditions, detonation wave has constant velocity of propagation through the explosive charge. If a steady-state is not achieved, than values of detonation parameters are changing. Such behavior is observed in the vicinity of the initiation sources, i.e. detonators. For successfully initiated detonation, values of detonation parameters will change towards steady-state values after certain distance from detonator. In order to investigate detonation behavior of an explosive, it is necessary to determine the influence of distance of detonation wave propagation on detonation velocity. In this research, cylindrical charges with five different double base propellants were initiated using electric blasting cap and spherical booster. Charges had 50 mm diameter and were made of paper or low density polyethylene. Boosters were made of 8 g of plastic-bonded explosive with PETN. Detonation velocities were measured at six different distances from detonator using measuring system with Tektronixő MSO2022B oscilloscope and electro-contact probes inserted inside of charges.

Destructive tests of the double-base propellant charge

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Keywords: double-base propellant; emergency situations; ballistic tests.

During the production of rocket fuels, reliability tests are conducted. These tests are to confirm the reliability of the product during its use. Sometimes, emergency situations may arise, for which special explanatory committees are appointed. The paper presents the results of research to explain the cause of one of the emergency situations.

Synthesis of bis(2-methyl-3,5-dinitrophenyl)diazene N-oxide from 2,4,6-trinitrotoluene

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Keywords: 2,4,6-trinitrotoluene; 2-amino-4,6-dinitrotoluene; NMR spectroscopy; thermal properties.

Bis(2-methyl-3,5-dinitrophenyl)diazene N-oxide was obtained in a two-step reaction starting with TNT. The reduction of TNT was conducted using iron powder and acetic acid. 2-amino-4,6-dinitrotoluene (2ADNT) was obtained via reduction and purified by crystallization from dichloromethane. Next, 2ADNT was oxidized with sodium hypochlorite solution. The final product was purified and analyzed by using the multinuclear NMR spectroscopy (^{1}H, ^{13}C, ^{15}N). The thermal properties and stability were determined by simultaneous DTA/TG techniques and were compared to the properties of commonly known energetic nitroaromatic compounds. Bis(2-methyl-3,5-dinitrophenyl)diazene N-oxide undergoes exothermic decomposition at 282řC. Furthermore, the heat of combustion was measured for the obtained compound and the enthalpy of creation was determined. The theoretical parameters of detonation were also calculated using a thermochemical code.

Prediction of detonation velocity of emulsion explosives sensitized by glass microspheres

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Keywords: emulsion explosives; the velocity of detonation; hollow glass microspheres.

The paper presented a novel algorithm and a computer code to predict the velocity of detonation of emulsion explosives (EMXs) sensitized by hollow glass microspheres. The detonation model of EMXs was based on Chapman-Jouguet hypothesis and the chemical equilibrium theory of explosion products. Obtained results show that theoretical values and experimental data of detonation velocity of EMXs including hollow glass microspheres in varying contents and diameters of explosive charge met good agreement.

Development of new eco-friendly solid rocket propellant

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Keywords: composite propellants; ammonium nitrate; polyurethanes; recycled PET; PSAN.

The paper deals with some theoretical and experimental studies regarding the development of new eco-friendly composites formulations, for rocket propellants, based on phased stabilized ammonium nitrate and different polyurethanes obtained by using various polyols including degradation products from recovered PET.

Sensitivity to impact for mixtures of okfol 3.5 with aluminum of various dispersion

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Keywords: impact; sensitivity; explosion; explosives.

The results of impact experiments on the weight drop-machine K-44-2 are presented to obtain data on the critical initiation pressures (Pcr) of mixtures of okfol 3.5 with aluminum of various dispersion - ASD-4 (8 μm), ASD-1 (15 μm), PA -3 (160 μm) and Alex (0,1 μm) in the entire range of component concentrations. It was found that at low aluminum concentrations (α <0.3), the Pcr values of the mixtures are almost the same (0,5±0,1 GPa), in the range of medium and high concentrations (0,3 <α <0,9), there is a slight difference in the behavior of the Pcr (α) curves in mixtures with micro-sized and large-sized aluminum particles. Mixtures with nanosized aluminum exhibit a significantly higher impact sensitivity. However, a certain relation between the sensitivity of the mixtures and the particle size of aluminum is not observed.

Nitrogen-rich Salts based on N-(5-(1,2,4-oxadiazol-3-yl)-1,3,4-oxadiazol-2-yl)nitramide: Synthesis, Characterization and Performance

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Keywords: energetic materials; oxadiazole; sensitivity; thermal stability; detonation performance.

Nitrogen-rich energetic materials have been studied widely for military and civilian applications. Development of energetic compounds with excellent detonation performance and low mechanical sensitivities is a long-term goal in the area of energetic materials. In order to investigate the detonation performance of combination of 1,2,4-oxadiazole and 1,3,4-oxadiazole and further explore new energetic materials, nitrogen-rich salts containing N-(5-(1,2,4-oxadiazol-3-yl)-1,3,4-oxadiazol-2-yl)nitramide anions with energetic cations (carbonic hydrazylhydrazidinium, guanidinium, aminoguanidinium, 1,2,4-triazolium, 4-amino-1,2,4-triazolium) were successfully prepared in high yield and purity. N-(5-(1,2,4-oxadiazol-3-yl)-1,3,4-oxadiazol-2-yl)nitramide was formed by the reaction of 5-(1,2,4-oxadiazol-3-yl)-1,3,4-oxadiazol-2-amine and fuming HNO3 at room temperature. 5-(1,2,4-oxadiazol-3-yl)-1,3,4-oxadiazol-2-amine was prepared in 4 steps by using readily available ethyl cyanoformate as the starting material. All the new compounds were fully characterized by FT-IR ,1H NMR, 13C NMR spectrometry, elemental analysis and differential scanning calorimetry (DSC), and their physical and energetic properties were investigated. Their heats of formation (HOF) and detonation properties (detonation velocity and detonation pressure) were computed by Gaussian 09 and EXPLO 5 program, respectively. Moreover, impact sensitivity (IS) and friction sensitivity (FS) were determined by standard BAM methods. These compounds exhibited high density, positive HOF, good detonation properties, low mechanical sensitivities and acceptable thermal stability. These results indicated that the combination of 1,2,4-oxadiazole and 1,3,4-oxadiazole provides a promising route to improve the properties of energetic materials.

Critical conditions of thermal explosion in a condensed system with dispersion of reactivity and stabilization of thermal decomposition of solid fuel

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Keywords: kinetics of heat release; dispersion of reactivity; thermal explosion; thermal decomposition of solid fuel; composition optimization.

A condensed system is considered in which monomolecular chemical reactions proceed and a dispersion of the reactivity of particles is present. To describe the nonisothermal kinetics of the system, a polychromatic mathematical model is used that contains the volume distribution function over ensembles of kinetically equivalent particles. The nonisothermal chemical process and the conditions for the occurrence of a thermal explosion substantially depend on this distribution function. Theoretically solved the problem of determining the critical value of the coefficient of heat removal. The problem of optimizing the stability of the system by minimizing the functional of the critical value of the heat removal coefficient over the distribution function of ensembles is posed as a natural problem for applications. An example of calculating the critical coefficient for real solid fuels is considered, its comparison is made with classical estimates of the zero-burn approximation according to Semenov and Frank-Kamenetsky.

Thermomechanical properties of heterogeneous propellants with burning rate modifiers

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Keywords: heterogeneous propellant; thermomechanical properties; DMA.

Thermomechanical properties of heterogeneous propellants were studied by Dynamic Mechanic Analysis (DMA) with two different modes: dual-cantilever and compression. The samples contained burning rate modifiers such as catocene and nano iron(III) oxide. The storage modulus, loss modulus, glass temperature and coefficient of thermal expansion were determined.

Development of a double stage small caliber gas gun for high speed impact testing

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Keywords: double stage gas gun; high speed impact; ballistic modeling.

The paper deals with the design and development of a double stage gas gun. The first stage of the gun used simple base gun propellant for piston propulsion, while for the second stage helium gas and metallic membranes were used. The calculus was performed in FLUENT environment and UDFs were specifically designed to describe the burning of propellant grains, their displacement inside the barrel and also the piston deformation in the truncated cone-shaped section. The interior ballistic model was validated by experimental tests.

Synthesis of the 3,6-Dinitro-[1,2,4]triazolo[4,3-b][1,2,4]triazolate Anion and Characterization of Its Energetic Salts

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Keywords: dinitrotriazoletriazole; energetic materials; explosives; heterocycles; high nitrogen compounds.

A new energetic anion 3,6-dinitro-[1,2,4]triazolo[4,3-b][1,2,4]triazolate (DNTT) is formed via nitro-Sandmeyer chemistry in a convenient and inexpensive three-step procedure from low-cost commercially-available starting materials. The utility of the DNTT anion in new energetic materials design is exemplified by the successful synthesis of several nitrogen rich salts. The chemical characterization (infrared, Raman, NMR, single-crystal X-ray) and energetic properties (impact, friction, thermal) of these insensitive energetic materials are reported.

Cellulose nitrates obtained from modified cellulose. Structure and properties

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Keywords: cellulose nitrates; IR-spectroscopy; low-substituted cellulose ethers; termogravimetry.

The consumption of cellulose products and its esters is increasing from year to year. Cellulose is a unique and indispensable polymer. Cellulose has a large raw material base and the presence of three hydroxyl groups in the structure of cellulose allows the production of cellulose ethers with various properties. The above qualities allow the use of cellulose in various industries: in the textile, food, pharmaceutical and defense industries. In addition, films, varnishes, plastics, linoleums, suspension stabilizers, filters, membranes, adhesives, etc. are obtained from cellulose and its esters. In this work, was studied the process of producing cellulose nitrates from modified cellulose by nitration with a triple acid mixture. The obtained cellulose nitrates were studied by IR spectroscopy, X-ray diffraction and differential scanning calorimetry, and the physicochemical characteristics of the obtained cellulose nitrates were studied. As a result of the work, it was shown that modified cellulose is a promising source of raw materials for the production of high-quality cellulose nitrates.

GC/MS/EI and HPLC/PDA studies on monitoring of a solid rocket fuel formulation based on ammonium perchlorate at controlled high temperature

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Keywords: antioxidants; solid fuel ageing.

Studies regarding the determination of two antioxidants, 2,6-di-tert-butyl-p-Cresol and Phenol, 2,2'-methylenebis[6-(1,1-dimethylethyl)-4-methyl, in a solid rocket fuel formulation based on ammonium perchlorate, aluminum and an inert binder, by high-performance liquid chromatography - photodiode array detection (HPLC/PDA) and gas chromatography – mass spectrometry in electron impact ionization mode (GC/MS/EI) have been carried out. Have been developed methods for GC/MS qualitative detection of antioxidants and HPLC/PDA quantitative measurements. Sample preparation and analysis procedures have been optimized during this study. HPLC and GC/MS determinations were performed after sonication-assisted extraction with methanol. These techniques were used for monitoring the variation of the concentration of the antioxidants from the solid rocket fuel, with time and temperature, during an accelerating ageing programme.

Physicochemical, molecular and detonation properties of nitro derivatives of carbamide and biuret

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Keywords: carbamide; biuret; nitro derivatives; molecular properties; detonation characteristics.

Results of a quite complete study of mononitrocarbamide, N, N'-dinitrocarbamide, mononitrobiuret and 1,5-dinitrobiuret are presented. The physicochemical properties of the substances were studied using methods of low-temperature X-ray diffractometry, infrared and Raman spectroscopy, nuclear magnetic resonance spectroscopy, elemental analysis and differential scanning calorimetry. Using thermogravimetric analysis and differential scanning calorimetry, thermal decomposition of materials was investigated, and using gaseous spectrometry and infrared spectroscopy, identification of gaseous decomposition products was carried out. The sensitivity of substances to shock, friction, and electric discharge was also determined. Molecular properties of these and about ten similar carbamide and biuret derivatives were determined using methods of quantum chemistry implemented in the Gaussian 09 computer code. The B3LYP hybrid functional and two basis sets of electronic functions, 6-31+G(d) and 6-311+G(2d,2p), were used in calculations. All geometric and energetic characteristics of molecules were calculated. The enthalpies of formation of molecules were calculated using the atomization method. The CBS-4M and CBS-3BQ calculating methods were used for that. The enthalpies of sublimation required to determine the standard enthalpies of formation were evaluated using an empirical method, which was calibrated on the base of calculated and experimental results for carbamide and biuret derivatives additionally considered. Possible primary decomposition mechanisms of molecules were considered and the activation energies corresponding to them were determined. Srystal structures of some of the substances under consideration and the properties of bound molecules were determined using the VASP computer code. The detonation characteristics of nitro derivatives considered were determined using the Explo5 computer code. The effects of detonation waves on barriers of several materials were calculated using the Ansys Autodyn computer code.

Molecular and energetic properties of tetrazole and a number of its derivatives

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Keywords: tetrazole; derivatives; molecular properties; enthalpy of formation; decomposition mechanism.

Results of a comparative calculation study of molecular and energetic properties of tetrazole and about forty its mono- and disubstituted derivatives are presented. The substances considered were 5-amino-1H-tetrazole, 5-methyl-1H-tetrazole, 5-phenyl-1H-tetrazole, 5-cyano-1H-tetrazole, 5-azido-1H-tetrazole, 5-nitro-1H-tetrazole, 1,5-diaminotetrazole, 5-amino-2-methyltetrazole, 1- methyl-5- phenyltetrazole, 5-vinyl-2-methyltetrazole, 1-amino-5-azidotetrazole, 1-amino-5-nitrotetrazole and many others. Molecular properties of all substances were determined using methods of quantum chemistry implemented in the Gaussian 09 computer code. The B3LYP hybrid functional and two basis sets of electronic functions, 6-31+G(d) and 6-311++G(2d,2p), were used in calculations. All geometric and energetic characteristics of molecules were calculated. The enthalpies of formation of all molecules were calculated using the approaches of atomization and isodesmic reactions. The CBS-3BQ calculating method was mainly used for that. The enthalpies of sublimation required to determine the standard enthalpies of formation were evaluated using an empirical method, which was calibrated on the base of calculated and experimental results for some of the substances most fully studied previously. The main primary decomposition mechanisms of molecules were considered and the activation energies corresponding to them were determined. For some molecules, their properties in ionized and excited states were also considered. For some of the most energy-intensive substances, the characteristics of their detonation decomposition and detonation performance were determined using the Explo5 computer code.

Molecular properties and energetic potential of furazanotetrazinedioxide and tetrazinotetrazinetetraoxide

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Keywords: furazanotetrazinedioxide; tetrazinotetrazinetetraoxide; molecular properties; detonation; combustion.

Results of a quite extensive calculation study of such high-energy tetrazine-based energetic materials as furazanotetrazinedioxide (1,2,5-oxadiazolo [3,4-e]-1,2,3,4-tetrazine-4,6-dioxide) and tetrazinotetrazinetetraoxide (1,2,3.4-tetrazino-1,2,3,4-tetrazine-1,3,6,8-tetraoxide) are presented. Molecular properties of all substances were determined using methods of quantum chemistry implemented in the Gaussian 09 computer code. The B3LYP hybrid functional and two basis sets of electronic functions, 6-31+G(d) and 6-311+G(2d,2p), were used in calculations. All geometric and energetic characteristics of molecules were calculated. The enthalpies of formation of molecules were calculated using the atomization method. The CBS-4M and CBS-3BQ calculating method were used for that. The enthalpies of sublimation required to determine the standard enthalpies of formation were evaluated using an empirical method. Possible primary decomposition mechanisms of molecules were considered and the activation energies corresponding to them were determined. The energetic potential of considered materials for their use in the processes of detonation and combustion was determined using methods of thermochemical and thermodynamic calculations implemented in the Explo5 computer code. In the case of detonation, all characteristics of detonation waves and the equations of state of detonation products necessary for gasdynamic calculations were determined. In the case of combustion, the energetic materials and their compositions with two types of binders were examined. The specific impulses and temperatures in the combustion chamber were calculated for adjusted pressures in the combustion chamber and at the nozzle exit. Shock wave loading of the barriers of several materials was considered too using gasdynamic calculation methods implemented in the Ansys Autodyn computer code.

Research on the explosive properties of N,N'-Bis-(1H-tetrazol-5-yl)-hydrazine (HBT)

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Keywords: nitrogen-rich explosive; N,N'-bis-(1H-tetrazol-5-yl)-hydrazine; HBT.

N,N'-Bis-(1H-tetrazol-5-yl)-hydrazine is an interesting example of so-called CHN type explosives. As its molecule does not contain any oxygen atoms, the detonation process is driven solely by its high enthalpy of formation. HBT was first synthesized by Thiele in 1898, but up to this day there is a lack of experimental data about its explosive properties. In this research, a scaled up process of HBT synthesis was developed, characterization of the product by various spectrometric methods was performed, and its various physicochemical properties were investigated. Finally, basic explosive properties such as VOD, critical diameter, pressure, and heat of detonation were measured.

Pyrotechnic time-delays: Al-Ni-NiO system

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Keywords: Thermite-Intermetallic System; Time-delay.

Pyrotechnic design flexibility is possible by combining classical thermites with intermetallic reactions. It offers the possibility of greener alternatives for current heavy metal-based compositions in some applications. High reaction temperatures are associated with conventional thermites and they can be lowered by the presence of an intermetallic system. Conversely, it is difficult to achieve sustained burning with intermetallic systems alone. To solve these problems, combination thermite-intermetallic systems are proposed. The concept is illustrated using the example of ternary compositions based on Al-Ni-NiO formulated as a time delay system. For example the stoichiometric mixture of the classic thermite reaction (2Al + 3NiO → 3 Ni + Al2O3) can be "diluted" by a stoichiometric intermetallic reaction system, e.g. (Al + Ni → AlNi). With this approach, it proved possible to reduce the adiabatic reaction temperature of the primary thermite by as much as 800 K while maintaining consistent burn behaviour inside glass tubes.

Determination of stabilizer content in naturally aged single base propellants

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Keywords: single base propellants; natural aging; stabilizer contect; chemical stability.

Information about the chemical stability of energetic materials is essential to a safe production, handling and disposal. Due to chemical reactions and physical processes that take place during the storage time, even under ambient temperature, a number of propellants properties may change. Methods for determining chemical stability can be used to predict life time and to choose the adequate storage conditions. Monitoring of stabilizer content is one of the reliable methods used to control chemical stability and predict the lifetime of a propellant. There are many studies addressing accelerated ageing at elevated temperatures, but there are few studies about long time ageing at ambient storage conditions. The aim of this work was to evaluate the chemical changes of single base propellant induced by natural ageing at ambient conditions during up to 55 years of storage. Tested material were 12 samples of single base propellants used for laboration of bullets with the caliber of 20, 82 and 100 mm caliber and manufactured between 1964 and 1990. The initial composition and the storage history of the studied propellants were unknown. The chemical stability was tested using HPLC, TLC, the vacuum stability test (VST), heat flow calorimetry (HFC) and the visual test with the Stereomicroscope. The results of diphenylamine (DPA) stabilizer concentration and its nitroso (N-NODPA) and nitro derivatives produced in propellants based on long storage showed that in three samples produced in 1990 and 1986 the initial stabilizer DPA was completely consumed (content <0.2%) and the VST value was > 2 ml/g, which classified these samples as unstable and unsafe for storage. Interestingly, another sample produced by the same manufacturer in 1986 showed effective stabilizer content of 0.59% but the VST value was > 3 ml/g, which also classified this sample as very unstable. The results showed that the changes in the tested samples were evident, although the results of the tests were rather scattered, which is a consequence of different ageing histories of propellants, measuring uncertainty or some other effects.

Evaluation of 1,5-dimethyltetrazole as a ligand in energetic coordination compounds

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Keywords: energetic coordination compounds; tetrazoles; structure elucidation; laser ignition.

Due to their capability to be initiated via laser stimuli, energetic coordination compounds gained a considerable amount of attention during the last decade. By combining different metal cations, energetic anions and ligands, the properties of those compounds can be easily adjusted to the intended use. In this study 1,5-dimethyltetrazole was synthesized by two different methods: a) reaction of acetone with azido(trimethyl)silane b) reaction of acetoxime benzenesulfonate with sodium azide. 1,5-Dimethyltetrazole was then reacted with the perchlorate salts of different 3d-metals (Mn, Fe, Co, Ni, Cu, Zn), in order to obtain new energetic coordination compounds. The resulting complexes were investigated by low-temperature single crystal diffraction experiments, complemented by EA, IR, DTA, sensitivity (impact, friction, and ESD) measurements as well as laser initiation tests.

Reducing the sensitivity of BCHMX by incorporating 2,2',4,4',6,6'-Hexanitroazobenzene (HNAB) in PBX mixture

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Keywords: explosives; nitramines; sensitivity; EXPLO5; performance.

The new eyesight in the fields of energetic materials is focusing on reserving high performance with enhancing the safety manipulation. In this work, special type of Plastic Bonded Explosive (PBX) mixture starts to be developed by combining new Nitramine, cis-1,3,4,6-tetranitrooctahydroimidazo-[4,5-d]imidazole (BCHMX), with thermally stable explosive 2,2',4,4',6,6'-Hexanitroazobenzene (HNAB), bonded by Styrene Butadiene Rubber binder. The studied PBX was prepared as an insensitive explosive and compared with the Czech plastic explosive (SEMTEX 10), new Egyptian Plastic Explosive (EPX-1) and with analogous PBXs, filled by RDX (1,3,5-trinitro-1,3,5-triazinane), β-HMX (β-1,3,5,7-tetranitro-1,3,5,7-tetrazocane), BCHMX , also individual Explosives; PETN, BCHMX, β-HMX and RDX. Impact and friction sensitivities in addition to the measured detonation velocities were obtained. The detonation characteristics were calculated using (EXPLO5 code). Different relationships between the performance and the sensitivity had been investigated. The results showed that BCHMX/HNAB-SBR has low sensitivity compared with the studied plastic explosives while its detonation characteristics are higher than the commercial plastic explosives.

Initiatives, activities and experience of Bulgarian MoD related to estimation and reduction of energetic materials impact on Army test range

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Keywords: energetic materials; contamination; environment; test range.

The pollution of environmental components on onsite training and test ranges became a growing problem nowadays, that focus the attention of governments and defence ministries worldwide. Within the majority of NATO and EU countries, a lot of different measures have been taken involving a vast number of an assessment of test ranges status and their current pollution content. A large number of recearches have been conducted in order to comprise distributing data on the measuted contamination levels of energetic materials and heavy metals in soil and grounwater. The constant use of munitions in those areas and the pollution, made by their constituents, put the problem of management of site contamination as an important one with the increasing international concern. The research has been executed at the Bulgarian test range Zmeyovo. From previous research project a method for extraction and quantitative identification of HMX, RDX, Tetryl, TNT, 2,4-DNT, 2,6-DNT, PETN and NG in soil, water and plants by HPLC with photo diode detection has been developed in accordance with EPA Method 8330B, EPA Method 8000 and EPA Method 3500. The developed method has been calibrated and validated. During the research different techniques have being developed to define the influence of physical and chemical properties, concentration, and distribution and residues of energetic materials in the soils to the current environmental status. Sample Analysis for energetic materials from soil, water and plants were made. The extracted samples were analyzed with HPLC for HMX, RDX, Tetryl, TNT, 2,4-DNT, 2,6-DNT, PETN and NG.

A new method for predicting heats of formation of energetic materials

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Keywords: heat of formation; energetic materials; bond enthalpy.

The ability to predict properties of energetic materials is a valuable asset for screening potential materials, particularly with regards to improving the safety for those working with these materials, as well as minimising chemical waste. The heat of formation of a gas phase molecule gives a reliable indication to the explosive power of the material, and thus is regularly employed for screening purposes. Currently, there are two common methods for calculating the formation energies of energetic materials. These are the use of isodesmic reactions, or the use of atom and group equivalent tools with electrostatic potential analysis. There are drawbacks to both methods; isodesmic reactions require good experimental heat of formation data for all other molecules in the reaction scheme, while analysis of the electrostatic potential of isolated molecules is limited to molecules representative of those used for training sets. This research aims to develop a new method for accurately calculating gas phase heats of formation of energetic materials using a fully computational approach. This method will be tested against a set of 10-15 CHNO energetic materials, for which the heats of formation are known experimentally, and have been calculated from other methods. The basis of this method is the use of a quantum mechanical calculation to obtain the force constants of individual bonds, which are directly related to the energy of each bond. The summation of the bond energies provide the gas phase heat of formation of the molecule. The feasibility of this new method will be discussed, and results will be compared directly against heat of formation values obtained from both isodesmic and atom equivalent procedures to determine its validity.

The properties of modified red flare pyrotechnic compositions

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Keywords: pyrotechnics; flare; illuminating; red; fireworks.

Red flare pyrotechnic compositions are commonly comprised of strontium nitrate, magnesium, chlorinated organics and binder. In this work different additives have been added to the optimized red flare composition in order to further increase it's light output while maintaining the low burning rate.

Urazine – a long established molecule and energetic chameleon

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Keywords: urazine; energetic material; X-ray; HEDO; HEDM.

Urazine is an easily accessible molecule from low-cost starting materials, still up to now it remained almost unnoticed in the energetic community. In this proceeding a colorful palette of reactions ranging from several new salt formations to complexations and condensations is shown. The structures of the resulting compounds were analyzed using X-ray diffraction studies, furthermore, the materials were thoroughly characterized using NMR spectroscopy, vibrational analysis, as well as elemental analysis. Vibrio fischeri - a marine bacteria - was used to determine the ecotoxicological impact of water soluble representatives. Depending on the field of application further investigations as energetic materials were carried out, including hot needle, SSRT, flame color and the estimation of the performance parameters using EXPLO5 V6.03 and Gaussian 09.

PETN – a sensitivity study

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Keywords: PETN; nitrate ester; drophammer; impact; friction; sensitivity; moisture; grain size.

Since accidents still happen on PETN plants, more information about the sensitivity of the nitrate ester is essential to ensure safer handling and transport. The sensitivity toward friction and impact of different PETN samples has been studied using the BAM Friction and the BAM Drophammer apparatus. The samples were modified and examined in their moisture, grain size and morphology. This was achieved by careful wetting, sieving and recrystallization from various solvents. The water content was determined by Karl Fischer titration.

Enthalpies of formation of derivatives pyrazoleazasidnones

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Keywords: calorimetry; enthalpy of combustion and formation; azasidnone group; nitro-pyrazole.

In the work first thermochemical study of a new class of energetic materials - pyrazole derivatives of azasidnon carried out. Combustion energy measure-ments are made on a precision combustion calorimeter specially designed to study energetic materials. The calorimeter allows to obtain results with high re-producibility on small attachments of the substance. As subjects of the study there are presented: (3-pyrazole-3-yl)azasidnone (I); 3-(1-nitropyrazole-3-yl)azasydnone (II); 3-(3-nitropyrazole-3-yl)azasydnone (III); 3-(4-nitropyrazole-3-yl)azasydnone (IV); 3-(3,5-dinitropyrazole-4-yl)azasydnone (V); 3-(3,5-dinitro-1-methyl-1H-pyrazole-4-yl)azasydnone (VI). Enthalpies of combustion and formation in standard state of tested compounds are calculated on the basis of half values of combustion energies. It was found that the enthalpy of the intro-duction of a pyrazole cycle into the azasidnone molecule increases the enthalpy of formation by 12 ÷ 30 kcal·mol−1.

Kinetics and mechanism of 6-R-gem-dinitro substituted 1,3-dinitro-1,3-diaza-5,7-dioxacyclooctane thermal decomposition

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Keywords: kinetics; mechanism; diazadioxacyclooctane; steric constants; correlation equations.

The structural-kinetic patterns and mechanism of thermal decomposition of 6-R-gem-dinitropropyl substituted 1,3-dinitro-1,3-diaza-5,7-dioxacyclooctane in the melt and solution of dibutylphthalate were revealed. The limiting stage has been defined for which the activation parameters are set and the entropy of activation is calculated. Between the decomposition rate constant, the activation energy and the steric constant of substituents R the quantitative dependencies have been found. These equations have a prediction of the thermal stability of unexplored compounds of this series.

Investigation of indium in pyrotechnical compositions

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Keywords: pyrotechnics; blue emitter; indium; flare.

High research efforts are driven towards finding environmentally benign blue light emitter in modern pyrotechnics. The in-use formulations apply copper and halogen sources to provide the blue-emitting species copper(I) chloride, copper(I) bromide or copper(I) iodide. For so-called "future pyrotechnics" there is a claim for halogen-free and more "greener" alternatives. The flame emission of indium as a potential halogen-free blue light emitter is discussed. Therefore, metallic indium was introduced as both fuel and colorant in various pyrotechnical formulations including guanidine nitrate or potassium nitrate as oxidizing agent as well as magnesium, hexamethylentetramine and 5-amino-1H-tetrazole as fuel. To the best of our knowledge, for the first time the flame emission of indium was investigated. Occurring emission lines of indium-based pyrotechnical formulations were recorded and evaluated.

Velocity of explosively driven copper and aluminum plates with identical mass

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Keywords: Gurney velocity; explosive acceleration; PDV; aluminium; copper.

A Gurney velocity is often used as to determine terminal velocity achievable by metal accelerated by explosive charge. The theory significantly simplifies the phenomena and does not include properties of the accelerated material. In this work we compare experimentally determined terminal velocities of copper and aluminum plates of exactly same mass accelerated by A-IX-1 charges and discuss the course of the metal acceleration. The experimental results are compared with results of Gurney approach and LS-DYNA numerical model for the same metal-explosive mass ratio. The velocity time histories were measured by photonic Doppler velocimetry.

Decomposition of ammonium dinitramide (ADN) elucidated by quantum chemical computations

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Keywords: computational chemistry; ammonium dinitramide (ADN); density functional theory; decomposition pathways; transition state structures.

Ammonium dinitramide (ADN) is a promising candidate as a green oxidizer to achieve minimum-signature of the exhaust gases of rocket propellants. However, stability issues and an erratic decomposition behavior limit its non-questionable general usability. This has initiated high research interest throughout the propellant community in order to optimize the ADN propellant system. Numerous experimental and theoretical investigations are revealing new aspects in the decomposition pathway up to this date. Here, we present a quantum chemical study based on density functional theory (DFT) exploring the initial decomposition reactions of ADN, its anion DN- and its acid HDN in vacuo as well as in aqueous solution. HDN exhibits several isomers with different protonation sites. These isomers lead to a multitude of transitions state structures towards the formation of HNO3 and N2O. We thereby identified a two-step reaction consisting of an isomerization with subsequent proton transfer due to a twist of the HDN molecule as the minimum energy barrier route towards HNO3 and N2O in vacuo. Alternative decomposition routes are presented and discussed. HNO3 is known to accelerate the decomposition of ADN autocatalytically. We investigate this effect by computing various clusters consisting of HNO3 and ADN related molecules ([HNO3_ADN], [HNO3_DN]- and [HNO3_HDN]) in order to establish an autocatalytic cycle. We complement our study by investigating the protonated, cationic species H[ADN]+ which may form in a low pH regime. We elucidate the influence of excess protons within the investigated molecule on the energy barriers of the decomposition pathways.

Regiodivergent assembly of high-energy isomeric nitrobifuroxans

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Keywords: Furoxan; high-density compounds.

Nitrogen-rich high-energy compounds comprising of two furoxan rings linked via C-C bond and additional explosophoric nitro and azido moieties were synthesized. The structure of prepared bifuroxans was confirmed by multinuclear NMR and IR spectroscopy. Synthesized furoxan derivatives have high nitrogen content and good oxygen balance. In addition, densities, thermal stability, impact and friction sensitivities of all compounds were determined. Enthalpies of formation and detonation parameters (detonation velocity and pressure) were calculated. According to our results, synthesized compounds have high densities, good thermal stability and high enthalpies of formation. Therefore, synthesized nitrobifuroxans may serve as promising ingredients for high-energy formulations.

Study of the initiating ability of salts of 5,5 ’-azotetrazole and their mixtures with oxidants

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Keywords: salts of 5,5’-azotetrazole with nitrogenous bases; mixtures with oxidants; transition of combustion to convective burning regime; transition of combustion to detonation; initiating ability.

Investigated the possibility of transition of deflagration to detonation salts of 5,5’- azotetrazole with the nitrogenous bases are: hydrazine, hydroxylamine, triaminoguanidine. It is shown that in the copper pipes in enclosed and semi-enclosed volume of the combustion of salts of 5,5’-azotetrazole of hydrazine and triaminoguanidine goes to the convective regime without transition to detonation. These salts do not possess the initiating ability for PETN. Only the salt of 5,5’-azotetrazole with hydroxylamine has the initiating ability, for which the minimum initiating charge for TNT is determined. We have investigated the possibility of transition of burning to detonation and initiates the ability of the coprecipitated stoichiometric mixtures of salts of 5,5’- azotetrazole with triaminoguanidine and ammonia with oxidizers - chlorate and potassium perchlorate. It is shown that the copper tubes in these mixtures there is a transition to convective burning regime without transition to detonation, as previously investigated individual salts. In contrast to the individual salts of 5.5’-azotetrazole, mixtures of salts of 5.5’-azotetrazole with triaminoguanidine and ammonia with the oxidant potassium chlorate have an initiating ability for PETN.

Recrystallization of BCHMX from different solvents

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Keywords: BCHMX; crystallization; explosives.

A relatively new nitramine cis-1,3,4,6-tetranitrooctahydroimidazo-[4,5-d]imidazole (bicyclo-HMX, BCHMX) is a very interesting compound in regards to high performance and rather cheap synthesis. In this work we made an effort to recrystallize BCHMX in order to obtain particles with good morphology and size distribution. The products were characterized with SEM and thermal analysis. The sensitivity towards friction and impact of the samples was determined.

Good balance between detonation performance and sensitivity: Research on molecule structure and performance of Fox-7-based High Energy Density Materials

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Keywords: FOX-7 derivatives; quantum chemistry; detonation performance; sensitivity.

Several new 1,1-diamino-2, 2-dinitroethene (FOX-7) derivatives are reported. These highly-oxygen and nitrogen-rich compounds were studied with quantum chemistry calculations and thermodynamics methods. Their optimized structure and detonation properties were firstly calculated and discussed under DFT-B3LYP method with 6-31++ G (d,p) basis set. After carefully comparison and research, among these derivatives, 2-3, 3-2 and 4-2 exhibit good performance as high energy density materials (HEDMs). Especially, 3-2 given outstanding value that is crystal density (2.05g/cm3) detonation velocity (10220m/s) and detonation pressure (48.47GPa) are even higher than those of CL-20 while its impact sensitivity (h50, 47cm) which remains a rather safety value compared with RDX's 33cm. Moreover, their synthesis routes, HOMO-LUMO orbitals and HOMO-LUMO energy gaps, electrostatic potential on surface of molecule, IR and NMR predicted spectra were also calculated.

Metal energetic salts based on 5,5'-azo-bis(1-oxidotetrazonate)with good thermal stability and sensitivity

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Keywords: metal salts; aot; sensitivity.

Some different kinds of metal energetic materials were prepared based on the nitrogen-rich ligand AOT (AOT: 5,5'-azo-bis(1-oxidotetrazonate)). All salts were fully characterized by differential scanning calorimetry (DSC), single X-ray diffraction, IR spectroscopy, and impact sensitivity. X-ray data indicates compound 1 is a 1D energetic coordination polymers with the density of 2.026g/cm3, while compound 2 and 3 are a kind of common salts with the density of 1.866 and 1.871g/cm3. From the single X-ray diffraction, it can be found that the compound 2 is very close to 3 in many aspects like the crystal structure, density and detonation performance due to the vicinity of Cu and Zn in the periodic table of elements. In addition, the detonation properties of these three metal energetic salts were calculated by EXPLO 5.05 which identify them as qualified energetic compounds.

Poly-nitro substituted dicyclic olefin: new high energy density materials with excellent detonation properties

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Keywords: high-energy density materials; dicyclic olefin; design; detonation properties; DFT.

In order to develop new high energy density materials, we designed a series of poly-nitro substituted dicyclic olefin. Based on the optimized geometry of the model compounds optimized at M062x/6-311+G* level, we evaluated its detonation properties and safety performance by a combination of semi-empirical and quantum chemical calculations. The results show that the compound 221-3b has a density of 2.01 g/cm3, accompanied by a detonation velocity of 9.91 km/s and a detonation pressure of 46.4 GPa, which is comparable to that of CL-20. While the compound 222-4a has an astonishing detonation velocity of 10.10 km/s and a detonation pressure of 46.7 GPa, which is one of the rare explosives whose detonation velocity exceeds 10 km/s. The safety performance especially the impact sensitivity of those model compounds was assessed. All in all, the poly-nitro substituted dicyclic olefin exhibit excellent detonation properties and are proved to be a new class of high energy density materials.

Copper(II) complexes of 5-nitrotetrazolate: An environmentally benign class of laser ignitable primary explosives

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Keywords: primary explosives; energetic coordination compounds; tetrazoles; laser ignition; sensitivities.

The requirements for the development of green primary explosives are well-defined: Main criteria are stability toward moisture, light, temperature, exposure to the atmosphere and tailored mechanical sensitivities. Additionally, no perchlorate or toxic metals must be present while maintaining a sufficient explosive performance. We have approached this task by utilizing the proven concept of Energetic Coordination Compounds (ECC) for designing several laser-ignitable primary explosives with high initiating efficiency. The novel complexes are based on copper(II) metal centers and 5-nitrotetrazolate anions, incorporating various nitrogen-rich neutral tetrazole ligands. All compounds were extensively characterized with analytical methods such as XRD, IR, EA, DTA, TGA and sensitivity measurements (IS, FS, ESD). The initiating behavior toward laser irradiation and their initiating efficiency were examined and compared to well-known explosives.

Single step synthesis of ANTA from 3,5-diamino-1,2,4-triazole using a common oxidizer

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Keywords: 3-amino-5-nitro-1,2,4-triazole; oxidizer.

3-amino-5-nitro-1,2,4-triazole (ANTA) is an insensitive explosive with performance greater than TATB and has received interest as a co-crystal and a precursor to other energetic molecules. In this paper, the synthesis of ANTA was reduced to a single step from 3,5-diamino-1,2,4-triazole under mild conditions using a commonly used oxidizer. The molecule was synthesized at the 1g-5g scale and a suite of analyses were conducted and confirmed that ANTA was the final product.

Energy of dissociation of N – NO2 bond in phenyl compounds

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Keywords: double difference method; enthalpy of formation; dissociation energies of bonds; aromatic compounds; 1- and 2-nitronaphthalenes.

On the basis of the enthalpy of formation in the gas phase of naphthalene derivatives, the enthalpy of formation of the radical naphth-1-yl and naphth-2-yl by the double difference method was determined. Using this value, the enthalpy formation of the 1-nitronaphthalene in gas phase was determined (133 kJ*mol-1). This value differs significantly from the data available in the literature (111.2 and 145.0 kJ*mol-1). For 2-nitronaphthalene 133 kJ*mol-1 in gas phase was determined; in the literature 129.8 kJ*mol-1. The obtained values allowed to estimate the dissociation energy of the C-NO2 bond in 1- and 2-nitronaphthalenes and compare it with the dissociation energy of the bond in nitrobenzene.

Synthesis and thermal decomposition kinetics of high-molecular weight poly(3,3-bis(azidomethyl)oxetane)

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Keywords: kinetics; decomposition; thermogravimetric analysis; 3,3-bis(azidomethyl)oxetane; polymer.

High-molecular weight polymer 3,3-bis(azidomethyl)oxetane was synthesized with a cationic ring-opening polymerization reaction in a solution using catalytic complex trialkilaluminium-water. Different aspects of thermal decomposition of poly(3,3-bis(azidomethyl)oxetane) were considered in the article. Kinetics of thermal decomposition was studied using thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) at 5, 10, 15 and 20 K/min heating rates. The calculation results of kinetics parameters, i.e. activation energy and reaction order, are given for single and multiple heating rate methods, namely Freeman-Carol, Coats-Redfern, Kissinger, and Flynn-Wall-Ozawa. IR-Fourie procedure, C, H, N-elemental analysis, and viscosimetry were used to describe all the compounds obtained.

A new method for the preparation of N-methyl-2,4,5-triniroimidazole

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Keywords: energy materials; N-methyl-2,4,5-triniroimidazole; synthesis.

The process for the preparation of N-methyl-2,4,5-trinitoimidazole (MTNI) has been improved. MTNI was synthesized from the imidazole, via a 4-tep sequence of reactions. The explosive performances were evaluated theoretically, and were found to be comparable to those of RDX and HMX.

Greening of pyrotechnic composition

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Keywords: pyrotechnic composition; non-toxic; REACH.

The paper deals with possibilities of substitution of environmentally unsuitable components in the production of pyrotechnic compositions. New compound of pyrotechnic composition must by comply with REACH requirements and be non-toxic. Heavy metal compounds will be removed. The "green" pyrotechnic compositions must retain all required pyrotechnic and ammunition characteristics.

Microcrystallites and detonation nanodiamonds granurality

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Keywords: detonation; synthesis; nanodiamond; microcrystalitte; granurality.

In science and technology, nanodiamonds of detonation synthesis, derived from both carbon molecules of explosives [1] and a mixture of explosives with the addition of graphite or soot, are used. In the latter case, nanodiamonds are larger [2]. This work examined fusion products obtained in industrial conditions during detonation from a mixture of trinitrotoluol with hexogen and hexogen with graphite. The size of microcrystallites was evaluated by X-ray diffraction analysis and particles granurality from the measurement of the specific surface area. The evolution of nanodiamond particle sizes, both in primary in fusion products and after enrichment from non-diamond carbon forms, is shown. The study was carried out with the financial support of the Russian Federal Property Fund in the framework of a scientific project No. 18-29-19070 MK.

Investigation of the relationship of mechanical characteristics, detonation parameters and sensitivity factors of energetic materials

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Keywords: energetic materials; explosives; elastic constants; mechanical characteristics; detonation parameters; sensitivity factors.

In this work, elastic constants and mechanical properties of PETN were calculated using DFT method with PBE functional taking into account the Grimme intermolecular interactions of D3(BJ) variant. The calculated elastic constants, mechanical properties and microhardness from ab initio calculations are in satisfactory agreement with the existing experimental data. The existing experimental elastic constants of ε-CL-20, PETN, RDX, β-HMX, FOX-7 and TATB were used to calculate its mechanical characteristics to find the relationship between it and the detonation properties and sensitivity of explosives. The dependences of the detonation parameters and sensitivity factors on mechanical properties of energetic materials were found. It is established that activation energy of explosive increases with increasing maximum value of the bulk modulus according to Voigt. Smoothly increasing function is also observed between the heat of detonation and microhardness. A decreasing function is observed between the impact sensitivity and microhardness. Formulas for predicting properties based on identified dependencies are proposed.

New applications of optical active method (OAM) for detonation measurements: detonation curvature and shock velocity induced on PMMA by seismoplast

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Keywords: optical active method (OAM); PMMA shock velocity; detonation front curvature; CJ pressure; seismoplast.

Detonation metrology is essential for development of energetic materials and for characterization of existing explosives. To accomplish these tasks, it is important to develop methods that uses short amounts of synthesized materials, which are easy to handle, not affected by magnetic fields and with an easy data analysis. The optical active method (OAM) is a detonation metrology based on PMMA optical fibers (250 ţm diameter), that receives continuously laser radiation with a centered wavelength of 660 nm and filtered by a window bandwidth of 650-665 nm. When the detonation wave (DW) or shock wave (SW) shocks the optical probe, the transmission properties of optical fiber is lost and the opto-electric radiation detectors observe an extinction of radiation. It consists on acquiring times from probes which positions are accurately known. These times are acquired when the laser radiation, which is constantly transmitted to the opto-electric converters, is interrupted due to the shock induced by the detonation wave on the optical probe. This method uses two kind of probes: the bare optical probes (BOP) and protected optical probes (POP). This paper pretends to show new applications of OAM with each kind of probe. With OAM-BOP it was possible to measure the shock velocity generated by seismoplast on different thicknesses of PMMA. It was measured the shock velocities in PMMA induced by seismoplast, using OAM-BOP, in different PMMA thicknesses (1 to 10 mm). The shock velocities on PMMA varied between 6346 and 4791 m/s and a set-up to determine shock velocity in inert materials was defined. The variation of shock velocity as a function of PMMA thickness allowed us to determine the CJ- Pressure of seismoplast. OAM-POP was used to visualize the detonation front curvature of seismoplast in charges with a rectangular cross section of 8x8 mm and with 8 probes.

Characterization of ADN droplets in a microfluidic process

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Keywords: ADN; ADN-prills; microfluidic processing.

Ammounium dinitramide (ADN) is currently the most promising oxidizer that has the potential to substitute ammonium perchlorate (AP) in solid propellants. The spherical shape of ADN (ADN-prills) is crucial for the incorporation in a propellant matrix. To investigate the crystallization behaviour of ADN-prills, a microfluidic emulsion crystallization method was developed, which allows the precise adjustment of the droplet size. To characterize the limits of the system concerning droplet size and droplet size distribution, five different system parameters were investigated and statistically evaluated.

Development of a powdered simulant for verifying X-ray detection of bulk TATP (triacetone triperoxide)

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Keywords: TATP; organic peroxides; explosive simulants; homemade explosives (HMEs); aviation; security.

This paper describes the development of a powdered X-ray simulant for the primary explosive TATP (triacetone triperoxide). The material matches the density and effective atomic number of a measured bulk sample of real TATP, and can be used to verify detection capability of baggage-screening equipment based on X-ray transmission.

Some aspects presented in Central European Journal of Energetic Materials on energetic output and effects

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Keywords: visual observation; detonation gases; blast wave; combustion front.

Some results and test methods are compared, upon the basis of data presented in papers published in Central European Journal of Energetic Materials. The main topic is determination of blast waves and combustion fronts. Presented data refers to the results of initiation of secondary explosives as well as pyrotechnic compositions.

Shock tube: activating and burning parametrs

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Keywords: maximal pressure; pressure rate; shock tube; activation.

Paper describe measurement of crucial parameters, which are needed for shock tube activation and stable burning in shock tube. These parameters are important for saffety functioning of shock tube. Shock tube is well known and established mainly for quarrying. However, the description of the burning processes in the shock tube is unsufficient. Function of shock tube is transfer activation impulse on the certain distance between donor and acceptor. It is made from multiple layers of different polymers, which are determine its mechanical properties. Shock tube is hollow and its inner wall is covered with coating of mixture Al/HMX. It has been on the market since the 1970s. The work is focused at the measurement of pressure and pressure rate, which are chosen as crucial parameters. These parameters were measured in different situation of activation or stable burning. First measured situation was stable burning condition. 2 meters long shock tube was used. Second situation was measurement of starting distance. It is distance, which is needed to reach stable burning. Variable lenght (0,1 to 4 m) of the tube was used. Last measured situation was innert gap. Results of innert gap measurement shown dependence of activation probability at lenght of shock tube segment without fill. Results shown basic pressure parameters, which are needed for activation and stable burning in shock tube. These informations are important for a thorough understanding of the burning processes in the shock tube.

Hybrids of heterocyclic compounds with cyclic nitramines

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Keywords: combustion; decomposition; kinetics; furazan; cyclic nitramines.

Nowadays there is a great interest to synthesis of hybrid compounds containing different heterocyclic systems in their structure. Some researchers consider that new properties could be caused by association of different heterocyclic fragments in one compound. In this research combustion behavior and thermal stability of 4,6,8-trinitro-4,5,7,8-tetrahydro-6H-furazano-[3,4-f]-1,3,5- triazepine, 4,6-dinitro-4,5,6,7-tetrahydro-tetrazolo-[1,5-a]-[1,3,5]-triazine and 4,5,9,10-tetranitro-4a,5,9a,10-tetrahydro-4H,9H-furazano-[3,4-b]-furazano-[3',4':5,6]-pyrazino-[2,3-e]-pyrazine were investigated. It was shown that furazan(tetrazole) heterocycle annelated with cyclic nitramines have decreased thermal stability due to weakening N-NO2 bond. Thermocouple measurements show that furazan cycle increases volatility of nitramines and decreases surface temperature. The reasons of observed phenomena are discussed.

Research of porous in pyroxylin porous and spherial powders by combustion models condensed systems with unrelated porosity

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Keywords: porosity; burning rate; condensed system; combustion temperature; spherical powders; propellant charges.

The article discusses the quantitative geometric model of a porous combustion system with unrelated pores allowing to predict the characteristics of its combustion in a wide range of pressures from the known laws of combustion of solid frame a porous system.

Searching for new thermostable energetic materials: synthesis and characterization of 5-acyl- and 5-sulfonyl-N3-(2,4,6-trinitrophenyl)-(1H-1,2,4-triazole-3,5-diamine) derivatives

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Keywords: high energy materials; explosives; 1,2,4-triazoles; nitrocompounds; 2,4,6-trinitrophenyl; thermostable energetic materials.

Nitrogen heterocycles are important building blocks in the synthesis of energetic materials. Azole based explosives exhibit not only good stability toward mechanical stimuli but also show increased thermostability. In this study, we present the synthesis of several new amide based nitroderivatives as potential candidates for thermostable energetic materials. Our convenient synthesis way is starting from 2-methoxy-1,3,5-trinitrobenzene. A subsequent controlled microwave-assisted aminolysis reaction with 3,5-diamino-1,2,4-1H-triazole represent a new synthetic procedure for the N3-(2,4,6-trinitrophenyl)-1H-1,2,4-triazole-3,5-diamine. Further reaction of the obtained 5-aminocompound with acylating agents lead to the synthesis of new energetic derivatives of 5-acyl- and 5-sulfonyl-N3-(2,4,6-trinitrophenyl)-(1H-1,2,4-triazole-3,5-diamine.The new synthesized compounds were characterized on the basis of HPLC-MS, spectroscopic methods, thermal analysis and flash points determination. The calculated energetic characteristics show that the new HEMs possess a perfect values, which are superior in comparison to the TNT. The data obtained from the thermal analysis and flash point investigation demonstrates a good thermal stability of these synthesized materials. On conclusion, the amide-based derivatization method may be useful for the thermostable materials design. Compounds, synthesized by this way, could serve as promising candidates for the application as thermostable explosives.

Prediction of Gurney velocity based on EXPLO5 code calculation results

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Keywords: Gurney velocity; Gurney energy; empirical model.

Output of an explosive is most commonly evaluated by the values of detonation velocity, detonation pressure and heat of detonation. These parameters can be determined experimentally or calculated by thermochemical codes. However, they do not answer the question how fast can an explosive accelerate surrounding metal liner. Important property, related to ability of explosive to accelerate metal plate or a liner, is described by R.W. Gurney. Gurney's model predicts the terminal velocity of explosively-driven metal liner on the bases of the mass ratio of metal to explosive and so-called Gurney velocity ($\sqrt{}$(2E_G)), which is a characteristic for a given explosive. The Gurney velocity is commonly determined experimentally by measuring velocity of cylinder wall, in so-called copper cylinder expansion test. Alternatively, it can be estimated based on certain detonation parameters. The accuracy of several simple empirical models are presented in the paper. The detonation parameters used in the analysis are calculated by thermochemical code EXPLO5. The Gurney velocities obtained experimentally are used to calibrate parameters in the models, as well as to validate the accuracy of prediction. It has been found that the model based on evaluation of the Gurney velocity from the detonation energy at relative volume corresponding to the terminal cylinder wall velocity (r0/r = 7) is superior to other tested methods. This method can predict the Gurney velocity of 41 tested explosives with the root mean square error (RMS) of 2.42%, while other tested models predict the Gurney velocity with RMS = 4.8 % - 7.9 %.

Identification of a series of nitrotoluene by the method of mass spectrometry of negative ions of resonant electron capture

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Keywords: nitrotoluene; negative ions resonance electron capture.

The identification of explosives, in particular trinitrotoluene, in various samples is essential for the implementation of counter-terrorism measures. One of the markers for the presence of explosives in the sample are reaction by-products - nitrotoluene. In this work, the method of fragmentation of the model group: mono-, di- and trinitrotoluenes, is analyzed by the method of negative ion mass spectrometry of electron resonance capture. For each test compound, characteristic negative ions were established. The work was performed on a serial quadrupole mass spectrometer coupled to a gas chromatograph. The data obtained are compared with studies previously performed on other types of mass spectrometers. For 2,4,6-trinitrotoluene, new fragmentary negative ions were formed that are formed upon resonance electron capture. Using data on the characteristic negative ions of nitrotoluene allows a targeted search for these substances in samples of various origins and an order of magnitude lower the lower detection limit of these compounds.

A study of the combustion behavior of metallized compositions based on KNO3 and Ba(NO3)2

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Keywords: inorganic nitrates; combustion behavior; propellant; aluminium; metal fuel.

The effect of metallic fuels on the combustion of compositions based on phenol-formaldehyde resin plasticized with dibutyl phthalate and KNO3 and Ba(NO3)2 with the same oxidizer excess coefficient, was studied. Two types of metal fuel were used: spherical Al powder (specific surface area 0.4 m2/g, average particle size 5.5 μm) and aluminium-magnesium powder (PAM) (mass ratio Al to Mg 0.83, specific surface area 0.24 m2/g, average particle size 12 μm). It is shown that Al and PAM introduction into the compositions by reducing the amount of oxidizing agent leads to the temperature increase and a change of the combustion products. The dependence of the combustion temperature of the studied compositions on the amount of metal fuel is extreme. With the introduction of metallic fuels into the composition, the burning rate increases and the dependence of burning rate on pressure decreases. This is due to the fact that the combustion of particles occurs in the diffusion mode due to their interaction with combustion products - H2O and CO2

Fluorescence quenching studies of energetic nitro compounds using BSA-polyaniline as fluorophore

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Keywords: doped Polyaniline; fluorescence quenching; energetic nitro compounds; resonance raman spectra; cyclic voltammetry: photoinduced electron transfer.

The trace detection of high energy materials (HEMs) is extremely important and more so in recent times. The fluorescence mechanism is understood from the interaction between the analyte (HEMs) with the benzenoid group of (Benzene sulphonic acid doped polyaniline (B-PANI). The doped PANI(B-PANI) has made the PANI highly processible eliminating the pi-stacking and thus facilitating easy detection of commercial explosives, i.e., RDX, Cl-20, PETN and scientifically intriguing next-generation explosives viz., Cl-20: RDX cocrystal. The quenching constant and LOD calculation have provided information on the sensitivity and selectivity to the trace level of detection of HEMs. The interaction between fluorophore and HEMs is studied from spectroscopy techniques employing FTIR and Resonance Raman studies, which show the presence of polaronic and bipolaronic group in the formation of a charge-transfer complex between HEMs and B-PANI undergoing PET mechanism predominantly. The cyclic voltammetry studies are undertaken and these studies collaborate with the fluorescence studies in understanding the possible fluorescence quenching mechanism from the electrochemical aspect.

Optimization of process parameters for production of low-nitrogen of cellulose nitrates

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Keywords: cellulose nitrates; solution viscosity; kinetics; mechanism; autoclave treatment; regression equations.

Analysis of influence of various factors on formation of cellulose nitrates properties (N = 11.9-12.3%) was carried out and original approach is presented, which provides creation of criteria of quality assessment and prediction of certain characteristics of product during high-temperature autoclave treatment on the basis of kinetic, as well as created regression equations. Analysis of parameters of technical properties of raw materials and nitrates themselves (low-nitrogen types of NC) allows to create regression models with the help of which it becomes possible to reduce a large number of sufficiently expensive and long-term tests and to obtain adequate models, which provide prediction of properties and control of the process of creation of NC with controlled and more homogeneous characteristics. In order to reduce the influence of moisture factor in cellulose, it may be recommended to maintain the weight fraction of water in the nitrated cellulose at (5 ś 0.2)% by introducing the cellulose drying step [1], or to use cellulose raw materials according to GOST 595 with guaranteed moisture value (5 ś 0.2)%. It is confirmed that the method of high temperature (autoclave) treatment of HC in a weakly acidic medium is most effective in reducing the viscosity of the HC solution. In order to optimize the technology of obtaining NC with uniform properties, the temperature modes of treatment in the autoclave should be correctly selected.

Syntheses of 15N-labelled nitro compounds with 2,4,6-trinitrophenyl group

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Keywords: nitroaromatics; 15N-labeled isotopes.

Syntheses of (15N3)-2,4,6-trinitrophenol, 1-chloro-(15N3)-2,4,6-trinitrobenzene and various nitro aromatics with (15N3)-2,4,6-trinitrophenyl group are described. Potassium (15N)nitrate was used as a source of (15N)nitro groups for starting (15N3)-trinitrophenol. The infrared and Raman spectra of the materials are evaluated, especially position and shift of (15N)nitro groups. The characteristic infrared frequencies of nitro groups are shifted in corresponding 15N- labelled isotopes.

Synthesis and characterization of 1-amino-4-nitro-1,2,3-triazole and 2-amino-4-nitro-1,2,3-triazole

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Keywords: energetic materials; explosives; N-amines; primary explosives; heterocycles.

Previously known 1-amino-4-nitro-1,2,3-triazole and 2-amino-4-nitro-1,2,3-triazole are characterized for the first time as energetic materials. Both compounds were characterized using NMR, Infrared, X-Ray, DSC, impact, and friction and found to be primary explosives with performances comparable to PETN.

New energetic coordination compounds based on the three different isomers of N-ditetrazolylmethane as ligands

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Keywords: energetic coordination compounds; primary explosives; laser ignition; ditetrazoles; structure elucidation.

The new ligands di(tetrazol-1-yl)methane, (tetrazol-1-yl)(tetrazol-2-yl)methane and di(tetrazol-2-yl)methane were synthesized and used for the concept of energetic coordination compounds (ECC). By varying the metal center and the corresponding anion the ECC's can easily be tuned toward their resulting performance and sensitivities. In the present study, the three different isomers were coordinated to different metal centers (e.g. Fe, Cu, Ag, Zn, Mn) as well as various anions (nitrate, (per)chlorate, and trinitrophenoles) and compared to each other. All complexes were characterized by XRD, IR, EA, DTA and sensitivity (impact, friction, and ESD) measurements. The most promising compounds were tested in classical initiation tests (nitropenta filled detonators) or irradiated with near-infrared light (NIR) laser diode which led to a reliable and safe ignition and expands their potential for future applications.

Synthesis and investigation of advanced energetic materials based on pyrazolytriazole backbones

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Keywords: pyrazoles; triazole; energetic; primary explosive; heat-resistant explosives.

Several energetic materials, which are comprised of pyrazole and 1,2,4-triazole backbones, were synthesized by a facile strategy and green cyclization method from 3,4-dinitro-1H-pyrazole-3-carboxyl into nitrogen-rich hybrids 3-(4,5-dinitro-1H-pyrazol-3-yl)-1H-1,2,4-triazol-5-amine (4) and 3-(4,5-diamino-4H-1,2,4-triazol-1-ium-3-yl)-4,5-dinitropyrazol-1-ide (6). Their molecular structures were fully characterized by vibrational infrared spectroscopy (IR), multinuclear NMR (1H, 13C) spectroscopy, elemental analysis. Additionally, the structures of 5 and 7-9 were further confirmed by single-crystal X-ray diffraction. The physicochemical and energetic properties for all energetic materials, including density, thermal stability and energetic performance were investigated. Among them, compounds 7-9 show high density (1.80-1.87 g cm-3), which is comparable to that of RDX (1.80 g cm-3). The thermal stability of compound 8 (314 řC) is comparable to that of HNS(318 řC). The calculated detonation veclocities (D) of compounds 7-9 (D: 8841-8923 m s-1) are superior to that of RDX (8795 m s-1). The good priming ability of compound 5 makes it a promising primary explosive.

Polynitro functionalized pyrrole derivatives: a new member of high energy density materials

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Keywords: high-energy density materials; polynitropyrrole; DFT.

In order to evaluate the potential of polynitropyrrole as an energetic compound with pyrrole as the molecular skeleton, a series of methyl, amino, nitro and hydrogen substituted pyrrole compounds were designed, and the molecular structures, energetic properties and safety performance were investigated by DFT method. The results show that more than three nitro-substituted pyrrole compounds have more energy level than TNT. N-NO_2 substituted pyrrole compounds have higher sensitivity than that of by C-NO_2 substituted. Among all the compounds, the predicted density of compound p9d is 1.963 g/cm^3, the calculated detonation velocity is 8.56 km/s, and the detonation pressure is 34.10 GPa, while the h_50 is just 3.0. The p9d is comparable to RDX. Generally, polynitro substituted pyrrole derivatives are expected to be a new member of high energy density materials.

Energetic salts based on cyclo-N5$^-$ anion: A comparative study of structure, physicochemical, and energetic properties

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Keywords: cyclo-N5$^-$ anion; energetic salt; crystal structure; performance.

Energetic salts based on cyclo-pentazolate anion and selected nitrogen-rich cations were prepared in highly yield by metathesis reactions. All new compounds were fully characterized by IR and multinuclear NMR spectroscopy, elemental analysis and TG-DSC measurements. The molecular structures of 2 and 3 were further confirmed by single-crystal X-ray diffraction studies. The sensitivities towards impact and friction were investigated using BAM standards. A detailed study based on x-ray diffraction was used to clarify the relationship between weak interactions and sensitivities of these energetic materials. In addition, heats of formation and detonation performances for all salts were evaluated using Gaussian 09 and EXPLO6 v6.01 programs, respectively. The synthesis and theoretical studies of these cyclo-pentazolate salts will play a pivotal role for constructing new energetic structures for practical use.

Synthesis and characterization of 5-substituted 1,2,4-triazole-3-methyl nitrate as potential high-performance energetic plasticizers

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Keywords: nitrate compounds; low melting; high-performance; energetic plasticizers.

This paper, the synthesis and characterization of nitro- and azido functionalized compounds, based on 5-amino-3-hydroxymethyl-1,2,4-triazole, for potential use as an energetic plasticizers is described. The azide group has a high positive heat of formation and it produces environmentally friendly nitrogen gas, the high oxygen content of the-ONO_2 group in nitrate esters provides an easily overoxidized potential and reduces the melting point of compounds. Therefore, the combination of an azide group and a nitrate group is beneficial to improve the performance of the triazole compounds. 5-Nitro-1,2,4-triazole-3-methyl nitrate and 5-azido-1,2,4-triazole-3-methyl nitrate as possible high-performance energetic plasticizers have been synthesized and characterized, and their physical and chemical properties have been explored. The all energetic materials were full characterized by IR, DSC and multinuclear NMR spectroscopy. 5-azido-1,2,4-triazole-3-methyl nitrate was additionally characterized by single crystal X-ray diffractometry. Energetic performance was calculated by using EXPLO5 v6.01 based on calculated heats of formation (Gaussian 09) and experimentally determined densities at room temperature.The impact and friction sensitivities were measured via standard BAM method. As a vital property of energetic materials, melting point determines the casting approach of explosives. According to the experimental results and computational analysis, the newly designed energetic materials have a good melting point and excellent detonation properties. Hence, the introduction of nitrate groups into high energy materials may be an effective pathway for designing and synthesizing potential energetic plasticizers.

Studies of the properties of RDX-based PBX with silicone binder

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Keywords: plastic bonded explosive; RDX; silicone binder; polydimethylsiloxane.

PBX with a fine RDX and silicone grease was prepared. The fine RDX was obtained by grinding in a ball mill filled with water. An approximate diameter of RDX particles was 2 microns. Silicone grease used in the composition was high viscosity polydimethylsiloxane. The following explosive properties of obtained PBX were determined: friction and impact sensitivity, shock sensitivity, temperature of decomposition, detonation velocity in different diameters, critical diameter, critical layer, heat of combustion, heat of detonation. The detonation parameters were also calculated using a thermochemical code. The experimental and theoretical data were compered. The analysis of the results leads to the conclusion that polysiloxanes may be useful components of PBX-type formulations. Further investigation may result in obtaining other interesting explosives.

Lead obsolescence in ammunition

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Keywords: REACH; lead bullet; toxicity.

Within the past years, a tremendous work has been performed to determine whether or at what extent lead is dangerous for the human health and for the environment. On September 12, 2018, ECHA recommended the restriction of lead in ammunition within the European Union. The impact of lead banning is obvious for the military environment, either while considering land, air or navy forces. Consequently, it is mandatory that lead substitutes to be found.

High density nitramine explosives assembling under 2D constraint materials

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Keywords: energetic materials; high density; crystal growth mechanism; 2D materials TAGP.

High energy content is considerable for energetic materials, newly researched high energetic materials still can not be widely used owing to high cost, sensitive, poor thermostability et al. It will make a big step if we can use 2D constraint materials assemble common traditional energetic materials such as RDX to get high density nitramine explosives. It has been shown that 2D TAGP layers provide a molecular level compression effect in RDX recrystallization process, resulting in a higher density packing of the RDX molecules. When RDX trapped in the 2D TAGP layers, the crystal growth can be easily influent by molar ratio of TAGP with RDX and solution. After assembling RDX with 2D TAGP, RDX crystals are free of defects, we can find perfect RDX crystals throw microscope or SEM, and melting endothermic peak decreased upon heating. The high density RDX also has higher heat of formation and better stability.

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