Abstracts of the 15th Seminar on

New Trends in Research of Energetic Materials

NTREM

Pardubice, April 18–20, 2012

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Institute of Energetic Materials

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Held at the University of Pardubice

Pardubice, Czech Republic
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Preface

In 1998, the management of Research Institute of Industrial Chemistry (belonging to joint-stock company Explosia) in detail dealt with professional level of its scientific research staff. A part of this consideration was to teach the young scientific researches of the Institute to present their research results in front of professional audience. Consequently the then director of the mentioned Institute, Dr. Miroslav Horáček, and leading scientist, Dr. Pavel Vávra, organized a seminar and invited also PhD students from the Institute of Energetic Materials (IEM) of the University of Pardubice to take part in it. The second seminar in 1999 was organized by IEM and was attended by a numerous groups of Polish colleagues. The third meeting in 2000 was attended by experts from the Czech Republic, Poland, Croatia, the Slovakia and England. The fourth seminar took place in 2001 and for the first time its official language was English. In this way began the tradition of international seminars NTREM, which was recollected in prefaces for the 5th (2002) and the 10th (2007) seminars and newly described in a monograph [1]. The following Table shows the trend of interest in participation in these meetings:

Seminar		Number of		
No.	year	countries	contributions	participants
3	2000	6	32	88
4	2001	11	41	106
5	2002	19	51	116
6	2003	18	60	129
7	2004	20	87	150
8	2005	22	106	160
9	2006	23	85	189
10	2007	23	108	199
11	2008	24	109	196
12	2009	27	99	195
13	2010	30	98	115*
14	2011	26	117	185
15	2012	22	100	180

* This 13th meeting was severely affected by Iceland's volcano eruption (April 16th, 2010) when air traffic was considerably reduced.

It may be mentioned here that simultaneously with our 15th Seminar NTREM other two meetings are in taking place elsewhere in the World; it is the 5th International Nitrocelulose Symposium in Spiez, Switzerland and Eleventh Zababakhin Scientific Talks in Snezhinsk, Russia.

One of the above-mentioned founders of the tradition of NTREM seminars, Dr. Pavel Vávra, joined IEM in 1998 as an Associate Professor. He belonged among significant representatives of Czechoslovak research into explosives and military technology. After a long and serious illness he died on Feb. 9th, 2012.

Realization of our Seminars would never be possible without the generous support from many institutions. The fifteenth NTREM seminar was financially supported by:

- U.S. Office of Naval Research Global, Middlesex, UK (conference grant)
- **U.S. Army Forward Element Command-Atlantic, Research Division, London, UK (conference grant)**
- Faculty of Chemical Technology, Pardubice, Czech Republic
- Austin Detonator, Vsetín, Czech Republic
- Indet Safety Systems, Vsetín, Czech Republic (member of the Nippon Kayaku group)
- OZM Reasearch, Hrochův Týnec, Czech Republic

The efficient help in ensuring smooth and successful course of the meeting obtained from all these institutions is gratefully acknowledged. I greatly appreciate that, thanks to this support, all specifics of the previous Seminars can be maintained. It would be quite unfair not to mention personal effort of our foreign friends helping to find funding, publicize the Seminar abroad and personally participate in organizing activities during the event.

And what should I add on the occasion of this jubilee 15th NTREM Seminar? Traditionally—first of all, I would like to express the wish: May its proceedings be successful and may it bring inspiration and pieces of knowledge for use in further scientific research activities in the area of energetic materials, may it enable establishing of new contacts and deepening of the existing ones particularly between the young participants in this meeting, and may the participants feel at home throughout the Seminar. Finally, I wish to 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 success 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.

[1] Zeman S., "Teaching of the Chemistry and Technology of Explosives in the Czech Republic". In: Armstrong R. W., Short J. M., Kavetsky R. A., Anand D. K. (Eds.), Energetics Science and Technology in Central Europe, Center for Energetic Concepts Development Science, University of Maryland, 2012.

Pardubice, March 15th, 2012

Svatopluk Zeman

In Memoriam of Associate Professor Ing. Pavel Vávra, CSc.

The Emeritus Associate Professor Ing. Pavel Vávra, CSc. of the Institute of Energetic Materials (IEM), Faculty of Chemical Technology died after a long and serious illness on February 9th, 2012. His decease means a loss of a colleague, friend and outstanding teacher valued by his students as a great personality whom they are indebted for key knowledge about the field of theory and practical applications of explosives. His humane approach, tolerance and ability to rise above problems gained him admiration and respect of all those who had come into contact with him. All of us will miss very much his commitment, openness, sense of humor and friendly nature.

Pavel was born in Prague on March 13th, 1936. He graduated from Department of Technology of Explosives (K102) of Military Technology Academy in Brno in 1959, whereupon he joined VCHZ Synthesia Rybitví and worked in the area of manufacture of basic nitro-, chloro- and amino-arenes. In 1963 he started to work at the Research Institute of Industrial Chemistry (VÚPCH) as a research worker in the field of synthesis of energetic materials. During his activities at this Institute he went through leading posts at the level of research group, department of primary explosives and finally as research manager.

The activities of VÚPCH were connected with research in the area of defense, which before 1989 meant virtual prevention of publishing of research results in open literature and complete isolation from colleagues in "non-socialistic" countries. Within "Eastern Bloc" VÚPCH was appraised as a top institute, and Pavel himself enjoyed high prestige from the side of the colleagues working at the respective institutes of Soviet Academy of Sciences. This was demonstrated, e.g., by the help of Russian experts with establishing of laboratory of polyfluorinated polynitro compounds in Pavel's group; it was one of only 14 workplaces of this type worldwide by that time. It is also possible to point out the esteem earned by Pavel from the side of the highly regarded scientist in the area of theory and practical problems of detonation, Professor Anatolii Dremin of the Institute of Chemical Physics Problems in the Soviet (later Russian) Academy of Sciences. Pavel (at that time as an Associate Professor at IEM) took over Professor Dremin's approach to explosion physics and introduced his findings into courses for our students. The defense of Pavel's dissertation thesis took place at the workplace of theory and technology of explosives, the University of Pardubice, in 1972, and the conferment of Associate Professor degree followed in 1997 at Military Academy Brno in the scientific area of Military Technology, Arms and Ammunition.

In 1979 he started his close cooperation with the above-mentioned workplace of explosives, later (1986) renewed Department of Theory and Technology of Explosives, University of Pardubice. In this department Pavel acted as a member of various expert committees and as external lecturer in courses of theory of explosives. In 1998 he joined University of Pardubice as an Associate Professor. He was supervisor of 10 PhD students, and his lectures about explosion physics were attended by 220 students at the MSc level and in licensed (retraining) study. He finished his work at the University due to bad health condition on December 31st, 2011.

Pavel Vávra's research work in VÚPCH was focused on synthesis of organic perchloryl compounds and polyfluorinated polynitro compounds and on study of relationships between molecular structure and

explosive parameters of energetic materials. Practical applications include active protection of armors on military vehicles and at IEM his participation in developing non-lethal defensive systems. Pavel's scientific activities at IEM brought a significant contribution to "relationships between crystal structure and sensitivity of energetic materials" published in two notable papers [1, 2] in cooperation with the team of Professor Petr Politzer of the University of New Orleans (Louisiana).

Professor Pavel Vávra was and remained a highly respected Czechoslovak doyen in the area of energetic materials and military technology, also favored for his above-mentioned humane qualities. His demise means a big loss for the whole Czechoslovak community of explosive and military technologies. Let us honor his memory.

[1] Pospíšil M., Vávra P., Concha M. C., Murray J. S., Politzer P., 2010, "A possible crystal volume factor in the impact sensitivities of some energetic compounds", Journal of Molecular Modeling, 16(5), pp. 895–901.

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Disposal Methodology of Composite Propellant with Civil Spin-Off Benefit of End Product as Fertilizer

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Keywords: composite propellant; safe disposal; liquid fertilizer; NPK; eco-friendly.

Large quantity of composite propellants is generated as waste due to life expiry of missiles / rejection of propellant lots during manufacturing. The environmental protection norm does not allow the hazardous materials for open burning/open detonation due to environmental and bulk hazards involved in these operations. Therefore, a systematic study has been carried out to develop a suitable method for the disposal of composite propellant into liquid product that possesses the nutrients useful for plant growth. In the present study, propellant compositions were digested in dilute nitric acid followed by neutralization with 5M KOH solution to get precipitated out aluminium as aluminium hydroxide and finally the liquid product was treated with orthophosphoric acid for further neutralization. The liquid product, thus, obtained was characterized for nitrate and phosphate content using ion chromatography while ICP-AES was used for the estimation of potassium, aluminium and other noxious metallic elements such as Pb, Cd, As, Cr, Cu, Ni & Zn. The analysis data indicate that liquid product is free from aluminium and noxious metallic elements while presence of nitrogen, phosphorous & potassium indicate the suitability of end product as plant nutrient (fertilizer).

Shaped charge jet initiation of explosives: a different view into penetration and initiation processes

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Keywords: explosives; penetration; initiation; shaped charge jet; modelling.

This paper's goal is to reveal to students and young researchers issues that could be more thoroughly examined through new experimental work on and modeling of the interface between a penetrator and a condensed explosive prior to its initiation.

In 1973, the author discovered experimental evidence revealing non-traditional concepts while he used shaped charges to penetrate tank ammunition in order to discover how to contain their destruction without injury to tank crewmen. This insight was used during the late-1970s to create devices for disrupting explosives without causing their detonation. The design rationale for these works was based on a non-traditional understanding of penetration processes – the "Kernel" model – and initiation of detonation by localized "hot spots" under combined pressure and shear. Although the "Kernel" model published in the Proceedings of the International Symposia on Ballistics is demonstrated clearly using experiments, the compressed stagnation zone is not found within conventional computational modeling when such modeling does not include true material viscosity. Thus, the "Kernel's" shear surface for initiation within an explosive is not currently clearly definable through modeling methods.

The proposed paper uses information from the above-mentioned publications and additional scientific literature to present a complete non-traditional overview of the physical processes tying together penetration and initiation processes. This overview offers insight into research areas that now can be explored more thoroughly by students using modern experimental and computational capabilities: ů Development and growth of the stagnated "Kernel" materials will be related to current views on the initiation of bare and covered condensed explosives, ů Acceleration of the "Kernel" piece from a cover through an air gap will be related to how an explosive charge is more sensitive when there is an air gap between a cover plate and the explosive, and ů Material motion within a condensed explosive will be related to how it affects the acceleration of the "Kernel" to a penetration velocity within the explosive and the formation of the explosive's stagnation zone forming the shear surface on which "hot spots" are most probably initiated.

Advances in the study of novel energetic materials

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Keywords: energetic powers; metals.

Some recent results from a project examining the use of novel energetic materials for structural components are presented. The aim of the research is to gain understanding as to how compressed metal powders could potentially boost performance in munitions casings. Specifically the experiments concerned involve loading rings of pressed tungsten-aluminium and nickel-aluminium composites using rubberised explosives in a copper container. The paper presents a number of insights into the experimental method and comments on potential material performance.

Low molecular weight components' influence on the effects of initial thermal decomposition of nitrocellulose based propellants

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Keywords: low molecular weight components; initial thermal decomposition; propellants; HFC.

In the present study was investigated the influence of low molecular weight components on the effects of initial thermal decomposition of nitrocellulose based propellants was investigated. Thermal stability studies were performed using a heat flow calorimeter TAM III. Two parameters were determined Qtransition, which is depended on the consumption of DPA and ttransition, which is depended on the amount of volatile compounds in propellants. Referring to the STANAG 4582 it was found that the propellants containing large amounts of volatile components and the propellants after removing these compounds using various methods are stable for 10 years at 25°C.

MEKP and Mixtures Containing MEKP: Chemical Investigation

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Keywords: peroxide explosives; MEKP; detection.

Solid peroxide explosives such as triacetone-triperoxide (TATP) and hexamethylene-triperoxide-diamine (HMTD) have been reported in a large number of illegal activities over the last decades because of their ease of preparation, their readily available ingredients and their reasonable performances. Consequently, they have been the focus of numerous technical and scientific investigations. A new kind of liquid non commercial explosive is currently potentially used: Methyl Ethyl Ketone Peroxide (MEKP). MEKP is an oily liquid synthesized from methyl ethyl ketone, hydrogen peroxide and catalytic amounts of acid. The product is a mixture of several dihydroperoxy-terminated oligomers, their proportion depending on the reaction conditions. Analytical procedures for the characterization, identification and detection of MEKP before and after explosion have been developed. Post-blast residues have been collected by wiping and the extract has been analyzed by liquid chromatography (LC) and gas chromatography (GC), both coupled with mass spectrometry (MS). The same GC parameters are used for a simultaneous analysis of TATP, DADP and MEKP in order to broaden the range of detection. Residues of MEKP have been recovered and detected after some explosions, using both LC/MS and GC/MS. The presence of residues depends on the ratio of MEKP in the original explosive mixture and on the type of explosive reaction (deflagration, low/high detonation).

Use of organic crystal structure prediction methods in the design of energetic materials

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Keywords: energetic materials; crystal structure predictions.

In the design of new of energetic materials (EM) the theoretical computational methods play still increasing role. EM are mostly organic solids, consequently, further efforts should be invested into the theoretical work aimed at predicting their solid-state structure and structure-based physicochemical properties. In particular, the nature of solid state effect on shock sensitivity of explosives can hardly be understood until proper theoretic models of relevant solid-state processes will be created. In this lecture, we review recent progress in the development of theoretical models, algorithms and computational tools that form together a kind of technology of crystal structure predictions (CSP) in the design of organic solid matter, such as EM are. The items to be discussed are as follows. Basic principles: molecular crystal structure models in terms of rigid molecular units; the structural classes of molecular crystals and their occurrence in organic matter; symmetry of potential-energy landscapes and the fundamental unit of global configuration space; local minima and stationary points. Systematic grid-based, stochastic and genetic algorithms of global energy minimization. Empirical atom-atom potential (AAP) models vs. 'first-principle' methods: their preferences and faults. Computer programs: PMC for global energy minimization of molecular crystal structures composed of flexible molecules; FitMEP for elaboration of point charge models from quantum mechanical 3D-distributions of molecular electrostatic potential; CRYCOM for numerical comparison of crystal structures in terms of cell deformations and rigid body parameters; FitPTL for refinement of empirical potentials on the basis of observed crystal structures and their physical properties. As to EM solids, a novel theoretical model of the pressure-induced phase transition in RDX will be presented. The key feature is that it describes successfully both changes in the crystal packing, involving the loss of crystallographic symmetry center, and changes of molecular conformation (from 'aae' type to an intermediate 'aae/aaa') on going from low to high pressures. An important field concerns verification and further improvement of intermolecular potentials with regard to new classes of energetic materials. On this matter, we report a calibration work on the atom-atom potentials of nitrogen in specifically the sp2 configuration. This work utilizes the known crystal structures of a series of purely N-aromatic heterocyclic compounds with no hydrogen bonds and a few available heats of sublimation. The model involves advanced point charge models of N-heterocyclic molecules which approximate accurately their electrostatic potential from ab initio calculation.

Energetic materials based on 3,5-diamino-1-nitroguanidine

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Keywords: nitroguanidine; tetrazoles; tetrazines; high explosives; crystal structures.

1,3-Diamino-5-nitroguanidine (1) was synthesized for the first time by hydrazinolysis of 1,3-dimethylmercapto-5-nitroguanidine. The synthetic protocol first yields 1,3-diamino-5-nitroguanidinium chloride (2) which can be deprotonated using alkaline bases to form neutral 1. The ability to form protonated energetic ionic compounds was verified by the formation of 1,3-diamino-5-nitroguanidinium 2-oxido-5-nitrotetrazolate (3). Diazotation of 2 with sodium nitrite yielded the two energetic compounds 3,6-dinitramino-1,2,4,5-tetrazine (4) and 1-amino-5-nitrimino-1H-tetrazole (5). Additionally, different nitrogen rich salts of 5 were synthesized and their energetic properties were explored. Compounds 1–5 were structurally characterized by low temperature single crystal X-ray diffraction. The sensitivities towards impact and friction were measured by BAM methods. Using theoretical (CBS-4M) heats of formation and the crystal densities several detonation parameters such as the velocity-, pressure, and energy of detonation were calculated with the EXPLO5.04 computer code. The compounds show great performance and could be used as starting materials for numerous new energetic ionic derivatives.

TKX50 and ABTOX - The revolution in RDX-replacements

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Keywords: 5,5'-bis-1-oxidotetrazolate; crystal density; detonation parameters; RDX replacement; sensitivities; thermal stability.

Two new high performing secondary explosives based on 5,5'-bis-1-oxidotetrazole, namely ABTOX and TKX50 have been synthesized in excellent yields in large quantities. They were completely characterized with respect to their chemical and energetic properties. Their calculated (EXPLO5.04) detonation performances exceed the performance of HMX and CL-20 (Vdet (TKX50) = 9687 ms-1, Vdet (ABTOX) = 9485 ms-1). Nevertheless, both show excellent thermal stability (Tdec (TKX50) = 221 °C, Tdec (ABTOX) = 290 °C) as well as compatibility in mixtures while being significantly less sensitive (IS/FS (TKX50) = 20 J/120 N, IS/FS (ABTOX) = 35 J/360 N) than commonly used explosives such as hexogen (RDX) and octogen (HMX). To study the initiation properties of both compounds, a small scale shock reactivity test (SSSRT) was performed. Here we observed performance (as evidenced by denting an aluminum block) after initiation of TKX50 comparable to HMX and superior to RDX.

Combustion Wave Structure of ADN-based Composite Propellant

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Keywords: ammonium dinitramide; combustion mechanism; burning rate; burning surface temperature.

Ammonium dinitramide (ADN) is high-performance solid oxidizer, however ADN-based composite propellant have high pressure exponent. Thus it is important to understand the combustion mechanism. Burning surface temperature measurement is the most useful method, but there is only one report about temperature profiles of ADN-based propellant. Reported results do not include pressure dependence of temperature profiles which is necessary to discuss about the combustion wave structure. It is also important to study about ADN, and there are a few reports about the burning surface temperature. However, detail mechanism on the condensed phase has not understood yet because more high time resolution measurements must be tried. Burning rates and burning surface temperature profiles of ADN/TP composite propellants were measured with fine thermocouples. TP stands for rubber-like thermoplastic polymer which was specially prepared in Japan. Burning rate jumps are found on the results of TP/ADN(20:80) and (30:70) at the critical pressure about 3.2MPa. The temperature profiles of TP/ADN(30:70) were measured under 1.3, 2.0 and 4.8MPa, and liquid phase is found under lower pressure than critical one. Temperature profiles of ADN with uncoated and coated ultra-fine (2.5micro-diameter) thermocouples. Voltage drop was found in the results of uncoated thermocouple, and they were suppressed by coated thermocouple. This fact shows the existence of ionic liquid phase on the surface. The temperature gradients became steep with decreasing the thermocouple diameter. The thickness of the condensed phase reaction zone and aerosol zone were estimated more accurately than reported one. The combustion wave model of ADN and ADN-based propellant can be made from these results and the simulation which includes the behavior of bubble and mists above the condensed phase will be presented.

Effect of charged and excited states on the decomposition mechanism of several peroxides molecules

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Keywords: peroxide; molecule; charged state; excited state; decomposition mechanism.

Peroxides find rather restricted practical application as explosives what is conditioned by the presence of a weak oxygen O-O bond resulting in low thermal and chemical stability and high impact sensitivity. For example, such well known peroxides as triacetone triperoxide (TATP) and hexamethylene triperoxide diamine (HMTD) are easily synthesized, are rather powerful primary explosives and possess the high sensitivity to heating, impact, electric discharge and intensive optical pulse. The results of studying properties of these explosives have shown that they can be utilized to create explosive compositions for laser initiation systems. The placement of these substances into a matrix of optically transparent polymers results in the considerable decrease of their impact sensitivity and corrosion activity by the maintenance of high sensitivity to the action of a laser pulse. The problems of laser initiation of explosives and understanding their sensitivity in general require knowledge of decomposition mechanisms not only in ground, but also in charged and excited states of molecules. In addition to mentioned two peroxides, the decomposition of more simple molecules of dimethyl peroxide (DMP) and diacetone diperoxide (DADP) was also examined. The electronic structures of all these molecules in different initial states were calculated at the B3LYP/6-31+G(d) level of theory. The ground states, positively and negatively charged states, and lowest triplet states were taken as the initial states of molecules. The O-O bond rupture was considered as the basic decomposition mechanism of peroxides. All potential energy curves while rupturing O-O bonds and possible transition states were determined for obtaining the energetic barriers of O-O bonds rupture reactions. It was observed that the lowest triplet state is the most unstable state with respect to the process of decomposition of all molecules. The negatively charged states are close to the triplet states being slightly more stable. The very low decomposition energy barriers and the high values of relaxation energies were marked for these states. On the contrary, the positively charged states of molecules are approximately as stable as their ground states.

Polynitropyrazoles as new green energetic materials: chemistry and thermal decomposition

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Keywords: thermogravimetry; differential scanning calorimetry; polynitropyrazoles.

Polynitropyrazoles are of great interest nowadays as new green energetic materials and because of their optimal set of energetic properties (density, oxygen balance, enthalpy of formation) and satisfactory safety. In this study, the thermal stability data of 3,4,5-trinitropyrazole and 3,4-dinitropyrazole obtained by the simultaneous thermal analysis (TG/DSC) are reported. Kinetic parameters of thermolysis were evaluated by model-free and model-fitting methods using TG-data. Theoretical predictions of mechanisms for thermal decomposition of synthesized compounds have been performed based on the results of activation energy (Ea) calculations (ab initio and DFT B3LYP/6-31G* methods) for computer-generated pathways. The results of calculations and experimental data are analyzed to evaluate the structure-thermal stability relationships for polynitropyrazoles.

"Green" energetic materials for primers

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Keywords: lead azide; lead styphnate; low toxic environmentally friendly primary explosives.

The problems of synthesis, properties and application of eco—friendly primary explosives have been discussed. Several prospective lead-free primary explosives were prepared and thoroughly studied during last decades. However manufacturing of modern "green" energetic materials on the industrial scale for practical applications in civil and military primers is the task of the nearest future

Theoretical investigation for adsorption of 2,4,6-trinitrotoluene on Al(111) surface

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Keywords: 2,4,6-trinitrotoluene (TNT); Al(111); adsorption and dissociation; density functional theory.

The adsorption of 2,4,6-trinitrotoluene (TNT) molecule on the Al(111) ultrathin film were investigated by the generalized gradient approximation (GGA) of density functional theory (DFT). The calculations em-ploy a supercell (4×4×2) model and three-dimensional periodic boundary conditions. The strong attrac-tive forces between oxygen and aluminum atoms induce the N−O bond breaking of the TNT. Subse-quently, the dissociated oxygen atoms and radical fragment of TNT oxidize the Al ultrathin film. The N-O bond of the o-NO2 group is easier to rupture than that of the p-NO2 group after the adsorption of the TNT molecule on the Al(111). Except for the breaking of the N−O bonds of the nitro group, other bonds of TNT molecule do not dissociate. The largest adsorption energy is -747.3 kJ/mol. The most of charge transfer is 3.42 e from the Al(111) to the fragment of TNT molecule. The aluminum ultrathin film is read-ily oxidized by the radical fragment of TNT, which is initiated by the dissociated O atoms from the nitro group.

Tautomeric equilibria and thermal decomposition of nitrogen-rich heterocycles: New insights from high-level ab initio calculations

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Keywords: tetrazole; thermolysis; ab initio calculations.

Nitrogen-rich heterocycles and their derivatives have recently attracted considerable attention as promising environmental friendly energetic compounds. Among them, tetrazole (TZ), 5-aminotetrazole (5-ATZ), and diaminotetrazole (DAT) are widely used building blocks for a huge family of novel high-energy species. The mutual interconversion and decomposition reactions of various tautomers of TZ, 5-ATZ, and DAT have been studied theoretically using various types of CCSD(T)/CBS procedures. The concerted double H atom transfer reactions in the H-bonded complexes led to fast equilibration between various tautomeric forms of the TZ, 5-ATZ, and DAT. The N-heterocyclic carbene isomer of TZ has never been considered before, however, it was predicted to be a key intermediate in the mechanism of thermal decomposition of TZ. In the case of 5-ATZ, new bimolecular reactions have been proposed to explain the experimentally detected formation of HN3. High-level computations allowed to reveal the role of tautomeric equilibria in thermal decomposition of TZ and 5-ATZ. The existing discrepancies in the mechanism and key intermediates of thermolysis of the title compounds have also been resolved. The calculated values of effective activation energy of TZ decomposition are in perfect agreement with the experimental data.

Evaluation of Ytterbium/Polytetrafluoroethylene/VitonTM as a Payload for Infrared Decoy Flares

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Keywords: Rare Earths; Pyrolants.

Pyrolants based on ytterbium/polytetrafluoroethylene/VitonTM (YTV) (87/10/3) exhibit volumetric energy density, Ev= 30 kJ cm-3, similar as those based on Magnesium/polytetrafluoroethylene/VitonTM (MTV) (60/30/10), Ev= 41 kJ cm-3 [1]. Thus YTV could in principle replace MTV in specialized decoy flare applications, provided the combustion energy transforms in a similar manner into useful radiation as with MTV. To check this hypothesis the intensity calibrated infrared spectra of various Yb/PTFE pyrolants were recorded. The combustion temperatures of the pyrolants were determined from the NIR spectra. To probe the radiation performance a number of Yb/PTFE/Viton formulations were prepared and tested radiometrically in two spectral bands in the infrared range [2].

Anomalies in influence of boron combustible content on the specific impulse

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Keywords: boron containing combustible; specific impulse.

A phenomenon of two maxima on the dependence "specific impulse = f (boron containing combustible content in energetic composition)" is investigated. It is shown that such an anomaly can appear at some ratios of CHNO-oxidizer enthalpy of formation, hydrogen content in boron containing combustible etc. At high content of boron containing combustible when there is not enough any more oxygen in the composition for B2O3 formation, the excess boron begins to form BN with nitrogen. In restrained terms it may increase specific impulse until all nitrogen is consumed

Measurement of blast wave intensity and blast wave overpressure of ammonal explosive

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Keywords: ammonium sulphate; ammonal; aluminum powder; blast wave.

This paper presents the results of measurements of detonation parameters (blast wave intensity and blast wave overpressure) for ammonium sulphate with different amount of sprayed and flaked aluminum powder. The experiment included application of sprayed and flaked aluminum (produced by Benda-Lutz-Werke) into ground ammonium sulphate. Blast wave intensity was measured by using Held's Method. Additionally the measurements of the blast wave overpressure were conducted with piezoelectric pressure probes equipped with pressure sensors PCB Piezotronics Inc. Series 137A. Positive effects of aluminum content on the blast wave performance and the blast wave intensity (work ability) of examined mixtures are also discussed.

Note on Determination of Relative Explosive Strength of Fortified W/O Emulsions by Means of Ballistic Mortar

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Keywords: ballistic mortar; emulsion explosives; performance; TNT.

Mixtures of W/O emulsion matrix and TNT have been prepared in the mass ratio of 1:1. The relative explosive strength (RS) of these mixtures was measured by means of a ballistics mortar. A concave relation was found between the RS values and grain size of the adopted TNT. It is stated that the course of this dependence is significantly affected by the sensitivity of the W/O explosives studied. This is also documented by the determination of shock sensitivity of the mixture with the TNT grains below 200 μm (2.53 GPa) and the grains above 1000 μm (3.75 GPa).

Biological degradation of nitrophenol mixture in a continuous aerobic reactor

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Keywords: mononitrophenols; continuous packed reactor; biodegradation.

This study is focused on the biodegradation of mononitrophenols (MNP) from a simulated wastewater in a continuously and long term operated packed bed reactor with immobilized cells (microbial consortium). At a hydraulic retention time of 45 min, the bench scale reactor was able to remove 2 g of the MNP mixture per liter per day (qw) with the removal efficiency (REw) of 99.5%. The position of the nitro group on the benzene ring strongly affected the rate and efficiency of the individual MNP isomers removal, when they were present in a mixture. Analyzing nitrite, nitrate and ammonium ions in the outflow water enabled us to predict the metabolic pathways of the individual MNP degradations. Monitoring of the microbial composition showed enrichment in Gram-negative strains with some fungal contamination.

"Green" energetic materials synthesis at LLNL

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Keywords: energetic materials synthesis; DNPP; llm137.

Abstract: The Energetic Materials synthesis group at LLNL is dedicated to the synthesis and scale-up of new energetic compounds with varying degrees of performance and sensitivity (safety factors). One of our main considerations during the synthesis scale-up phase is ensuring that the synthetic scheme is as environmentally benign as possible, mainly through the elimination of toxic and carcinogenic starting materials and solvents, reducing the number of synthetic steps, and improving product yields and purity. In addition we synthesize high-nitrogen compounds such as 4,5-di(tetrazol-5-yl)-1,2,3-triazole (LLM-137) as "green" energetic compounds. In this paper several examples of "greener" Energetic Material (EM) syntheses, including new synthetic schemes to 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105), 3,6-dinitropyrazolo[4,3-c]pyrazole (DNPP) and 3,4-bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole-2-oxide (BNFF) will be described.

Phytoremediation of Nitroglycerine by Aquatic Macrophytes and Wetland Plants

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Keywords: phytoremediation; nitroglycerine; aquatic macrophytes ; wetland plants.

Present and historical methods for the disposal of munitions (explosives & unexploded ordnances) which include open burning/ detonation, burial and controlled incineration are unacceptable due to environmental concerns. The aim of this study is to assess the feasibility for phytoremediation of a widely used explosive nitroglycerine (NG) from water using two commonly available aquatic macrophytes and two wetland plants viz. Eichhornia crassipes (Water hyacinth), Pistia stratiotes (Water lettuce), Typha latifolia (broadleaf cattail) and Phragmites australis (common reed). Hydroponic studies were conducted to determine the plant's capability to remove the contaminant NG present in the water. The percentage uptake of NG and the subsequent biochemical changes appear in the macrophytes and wetland plants on exposure to NG were studied with the starting concentration (80 mg/L) capable to inhibit the growth of plant up to 50%. The extracts of plant's root and shoot were analyzed by FTIR, HPLC and GCMS to understand NG migration and its degradation. NG was found readily taken up by Typha, Phragmites, Eichhornia and Pistia in hydroponic experiments and the NG concentration is remarkably reduced (> 50%) after exposure of 5 days for all the system. The analysis of roots and leaves extracts of Phragmites, Eichhornia and Pistia at different time intervals indicates the accumulation of NG with marginally higher concentration in the leaves than that of in the roots. No accumulation of NG was observed in the tissues of Typha after 48 h. The total NG accumulated in leaves and roots of the Eichhornia and Phragmatis system are found to be 15.2±1.5% and 5±2.8% respectively of the initial NG taken for the study. The observations of biochemical profile, the NG accumulation in the root tissues and its translocation to leaves conclude that the Typha latifolia is the best among four systems for phytoremediation of NG. Keywords: Phytoremediation, Nitroglycerine, Aquatic Macrophytes and Wetland Plants

MEKP and Mixtures Containing MEKP: Detonics Investigation

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Keywords: MEKP; peroxide explosives; sensitivity; explosives performances.

For many years, solid peroxide explosives and liquid explosives have been the target of many scientific investigations as a consequence of their use in illegal activities. The liquid peroxide Methyl Ethyl Ketone Peroxide (MEKP) is since a couple of years on the list of such explosive material. In this paper, in the continuity of the study of the chemical properties and detection of MEKP (see paper entitled "MEKP and Mixtures Containing MEKP: Chemical Investigation"), we investigate the explosive and detonics properties of MEKP. The investigation focuses on sensitivities, initiation capability and performances, in order to assess the potential hazard and (mis)use of this energetic compound, first as pure material but also as ingredient in various energetic mixtures. MEKP turns out to be an extremely sensitive material, specifically to impact. As main explosive charge, pure MEKP exhibits relatively poor detonics performances, but its impregnation on a solid material with high oxygen content, such as ammonium nitrate (AN), produces a high energetic formulation. Note that the combination of ammonium nitrate with other energetic materials has been largely used in recent years in terror actions. Experiments performed at laboratory-scale indicate that mixtures MEKP/AN in adequate proportion may be detonated with adequate thermally initiated devices.

Comparative Study of Combustion Mechanism of Guanidine Salts: Triaminoguanidine and 3,6-Diguanidino-1,2,4,5-tetrazine Nitrates

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Keywords: triaminoguanidine nitrate (TAGN); 3,6-diguanidino-1,2,4,5-tetrazine nitrate; combustion mechanism; decomposition; kinetics.

Triaminoguanidine nitrate (TAGN) is considered as a perspective component for some gun powders, gas-generating compositions and "green" (free of HCl-containing exhaust gases) double-base and composite propellants. It is also offered as an effective activator and burning rate modifier for ammonium nitrate (AN) based propellants containing high energetic nitramines. In recent years, attention of researchers has been also addressed to 3,6-diguanidino-1,2,4,5-tetrazine nitrate (DGTN). This compound is considered as a low-sensitive explosive. Both compounds have the same structural fragment: the protonated guanidine moiety, which allow suggesting the close combustion mechanism. The goal of the present work was to study the TAGN and DGTN combustion behaviors, their combustion wave structure and to determinate the location and chemical nature of the leading reaction on combustion. Burn rate measurements were carried out in a constant pressure window bomb with a volume of 1.5 liters. A video camera was used to determine the character of the combustion process as well as the burning rates. The mixtures under investigation were placed in transparent acrylic tubes, 7 mm in diameter and 12-15 mm long. Temperature profiles in the combustion wave were measured using P-shaped thin (7 mm) tungsten-rhenium thermocouples. The thermochemical data of the decomposition process of TAGN and DGTN were obtained with DSC analysis. DGTN in the form of samples pressed into acrylic tubes can sustain stable combustion at subatmospheric pressure. In the pressure range 0.1-10 MPa DGTN burns 1.5-2 times faster than HMX, but 2-3 times slower than TAGN. The burning rate of TAGN grows steadily as the pressure increases up to 2 MPa, showing the pressure exponent of 0.94. A kind of burning instability region sets in then, characterized by the constant burning rate, which begins to increase again at pressures higher than 4 MPa. Thermocouple measurements show the close surface temperatures for both salts. It was shown that combustion of both substances obeys the condensed-phase mechanism. The higher burning rate of TAGN connected with the higher decomposition rate in the melt layer. The kinetic parameters of the controlling chemical reaction have been estimated, and the detailed combustion mechanism of TAGN and DGTN has been proposed.

The Influence of Calculation Accuracy of Formation Enthalpy and Monocrystal Density Estimationson Some Target Parameters for Energetic Materials

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Keywords: formation enthalpy; density of monocrystals.

The set of schemes to estimate the enthalpy of formation and molecular crystal density has been considered. There were some additive schemes, QSPR-approach (Quantitative Structure-Property Relationships), ANN-method (Artificial Neural Networks), the method of AAPF (Atom-Atom Potential Functions). For compounds from different chemical classes the accuracy of estimation some basic parameters has been considered and the influence of this accuracy upon ballistic parameters and specific impulse has been evaluated.

Laser induced breakdown spectroscopic studies of HEM's using nanosecond and femtosecond pulses

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Keywords: LIBS; nanosecond; femtosecond.

We present our results from laser induced breakdown spectroscopic (LIBS) studies of NTO, HMX, and RDX investigated using nanosecond and femtosecond pulses. The presence of C, CN peaks in the LIBS spectra, signatures of high energy materials, was confirmed and their lifetimes have been measured. The number of Nitrogen peaks was found to be higher in the ns spectra. The presence of an additional CN peak in the fs spectra was detected for all the samples. The ratio of CN peak (388.28 nm and 387.08 nm) to C (247.82 nm) was discovered to be stronger in the fs LIBS spectra.

Some chemical properties of 3,4-bis(3-nitrofurazan-4-yl)furoxan

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Keywords: 3,4-bis(3-nitrofurazan-4-yl)furoxan; azepine.

The results of our studies of reactivity of 3,4-bis(4-nitrofurazan-3-yl)furoxan (BNFF) con-cerning the action of some O- and N-nucleophiles are presented. It is shown that both nitro groups of the above compound can be easily replaced by nucleophile. Depending on used nucleophile BNFF may be transformed to two types of 1,2,5-oxadiasole derivatives, notably 4-R substituted bis(4-R-furazan-3-yl)furoxanes or 7-R substituted 7N(7R)-tris[1,2,5]oxadiazolo[3,4-b:3',4'-d:3",4"-f]azepine-1-oxides - a new heterocyclic system including azepine ring annelated with three 1,2,5-oxadiazole rings.

Compaction behaviour of ammonium nitrate prills

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Keywords: ammonium nitrate; drop weight; compaction; Kawakita model.

The compaction behaviour of a range of commercially available ammonium nitrate prills was studied in two different strain-rate regimes. Confined beds of diameter 13mm, length approximately 15mm were compacted by a piston. This provided pressure-porosity data. In the low strain-rate regime, approximately 10^{-4} s^{-1}, the piston was driven using a screw-driven instrumented press. Pressure was calculated using a load cell, while porosity was inferred from the known motion of the driving screws. In the high strain-rate regime, approximately 100 s^{-1}, the piston was driven using a drop weight. Pressure was again calculated using a load cell. The motion of the weight was tracked using a line-laser occlusion system, allowing porosity to be inferred. For all prill types, the bed offered increased resistance to compaction in the high strain-rate regime. It was also found that prills with denser microstructures offered greater resistance to compaction than those with less dense microstructures. The beds' behaviour suggested that the primary mechanism of compaction was plastic flow of ammonium nitrate. The Kawakita compaction model, which has been successful in fitting the pressure-porosity curves for agglomerates of soft pharmaceuticals, was found to fit the pressure-porosity data well.

Boron – Viton Based Fuel Rich Propellant Processing

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Keywords: fluorocarbon; binder; powder compaction technique; UCS; safety parameter.

Boron is a preferred metal in air augmented propulsion because of its very high heat of combustion per unit mass and per unit volume. It is also known for its poor combustion because of oxide layer (B2O3) formed on its surface which inhibits the combustion of boron. Many methods, such as incorporation of magnesium/aluminum (MA) alloy, coating of boron particles with metal fluorides, use of fluorinated oxidizer, use of fluorocarbon binder are reported to improve the combustion of boron. Use of fluorocarbon binder can be a promising approach for the improved ignition of boron. In the present study Fuel Rich Propellant (FRP) composition based on Boron as a fuel / Ammonium Perchlorate (AP) as an oxidizer / vinylidene fluoride, hexafluoropropylene and tetrafluoroethylene terpolymer (Viton-B) as a fluorocarbon binder is processed. The binder percentage is one of the main parameter which governs the mechanical properties and density of FRP. For binder percentage studies, different compositions of propellant are processed using 10, 15, 20 & 25 percent of Viton-B and it is compensated by Naphthalene as total percentage of binder in the propellant composition is fixed at 25 percent. The propellant grains are made by Powder Compaction Technique (PCT). These grains are used to evaluate mechanical properties like ultimate compressive strength (UCS), % Compression and Modulus by Universal Testing Machine (UTM) following ASTM standard D695-02A. Density is determined using Archimedes principle. Propellant composition is characterized for safety parameters like impact sensitivity, friction sensitivity, spark sensitivity and auto ignition temperature. Impact sensitivity is evaluated by 2 kg Fall Hammer test and sensitivity to friction is determined by Julius Peters apparatus. It is found that as the percentage of Viton-B increases from 10 to 25 percent, the mechanical properties values like UCS increases from 114 to 160 kgf/cm2 and % Compression from 10 to 25; and density increases from 1.44 to 1.82 g/cc. Safety parameters are found insensitive to percentage of Viton B. It is found that height of 50% explosion is 58 cm, Figure of Insensitivity is 70, auto ignition temperature is 360oC and composition is insensitive to friction up to 36 kg and to spark up to 5 Joules. From the present study it is concluded that Boron based FRP having Viton as a binder is safe with good mechanical properties and high density.

Relationship of rheological properties and stability of emulsion matrix

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Keywords: emulsion matrix; rheological properties; surface tension; double yield phenomenon; linear elastic region.

Please fill in (or paste) your abstract here. Use about 300 words.

Abstracts: Emulsion explosives are one of the important industrial explosives. Stability of emulsion explosives determines its reliability being initiated, safety and detonation performance in use. Moreover, emulsifier is one of the most important factors affecting stability of EM(emulsion matrix) and EE(emulsion explosives). In this paper, several emulsifiers with amide, imide, ester and SMO functionality were selected. From the view of rheological properties, effects of emulsifier structure and functionality on viscosity and visco-elastic properties were analyzed and researched. The results show that emulsifier with amide, imide functionality and corresponding emulsion matrix has higher viscosity at normal temperature and better fluidity at high temperature than that of other. Linear viscoelastic region for emulsion matrix by the emulsifier is larger. Effect of the change of ambient temperature on the viscosity for mixed emulsifier decreases. Compared with the results of surface tension and high-low temperature cycle experiment, emulsifier with high viscosity, high elasticity modulus, a large LVR has large surface tension and more cycle number. Corresponding storage stability is much better than others. The emulsifier is very suitable for packaged emulsion explosives, while emulsifiers with SMO and ester are the best choices for emulsion explosives filling on site. Keywords: emulsifier; emulsion matrix; rheological properties; viscoelasticity; stability

Combustion Behaviour of Gelled Nitromethane Propellants Filled With Metallic Particles and Hydrides

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Keywords: gelled propellants; metal combustion; thermite reaction.

Gelled propellants combine the advantages of solid propellants which do not pour out on leakages with those of liquid propellants which are pumpable and burn well-defined in sprays. In many applications gelled mono-propellants offer essential advantages according to system design, ignition and combustion. Nitromethane (NM) is a promising candidate to be used as green gelled mono-propellant for rocket propulsion. To enhance the performance metallic or other pyrotechnic particles may be added. In this study NM filled with particles of Al, B, Mg, Si, Ti and Zr as well as AlH3 and MgH2 was investigated. The burning behaviour of gelled NM including fumed silica and mixed with 10% of metallic filler was investigated under pressure from 2 to 13 MPa in a window bomb to determine burning velocity and combustion temperature. In all tests, stable and self-propagating combustion were found resulting in increased burning velocities and improved ignition behaviour. In many cases the burning velocity shows a kind of mesa-effect at about 6 to 8 MPa that is close to the critical pressure of nitromethane. The replacement of aluminium and magnesium by their corresponding hydrides does not increase the specific impulse but improves the burning behaviour and results in lower combustion temperatures. The investigations also show that metal filler particles of e.g. Al and Mg react exothermic with fumed silica. This is in contrast that this widely used gelling agent is usually considered as inert. The experimental study was completed by the observation of the combustion of single droplets on a red glowing plate inside a Bunsen flame. These investigations show that in most cases the metallic reaction does not start before nitromethane is largely evaporated.

Study on the combustion behavior of metalized double-base propellants (III): Heat effects of the metals on the burning rate and flame temperature

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Keywords: double-base propellant; reactive metals; combustion; flame structure; heat effects.

The combustion properties of double-base propellants containing reactive metals such as aluminum (Al), magnesium (Mg), boron (B), nickel (Ni) and Mg-Al mechanical alloy (Mg/Al=3/4) are investigated by means of burning rate test, high-speed photography technique, Non-contact Wavelet-based Measurement of flame temperature distribution, Scanning Electron Microscope (SEM) and Differential Scanning Calorimetry (DSC). The research investigates how the heat effect of the metals in condensed phase and gas phase controls the burning characteristics of double-base propellants containing such reactive metals. It was indicated that the heat effect of the metals by conduction in solid phase, by change of phase consisting of both evaporation and condensation in the interphase and by radiation in gas phase are considered to provide a complete description of the heat transfer process in the combustion of metalized double-base propellants, and the combustion process of them are mainly involved with the oxidation of the metals and thermolysis of NC/NG and RDX. In combustion of aluminum, magnesium, and Mg/Al in solid propellant, there are gas phase reactions and also surface oxidation resulting in volatile and non volatile products which include oxide and suboxide species. However, there are only gas phase reactions for boron and transition metal nickel due to the higher melting point and enthalpy of vaporization. A mathematical model of heat transfer by radiation for the propellants containing reactive metals has been theoretically and experimentally established and analyzed. It was concluded that the B-MDB and Al-MDB propellants are of the higher theoretical radiation heat which in practice are converse due to their agglomeration and incomplete combustion.

Theoretical study on novel nitrogen-rich energetic compounds with tetrazene unit

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Keywords: 5,5'-bis(amino)-1,1'-azobis(tetrazoles); stereoisomers; electronic structures; heats of formation; energetic properties.

Six stereoisomers of 5,5'-bis(amino)-1,1'-azobis(tetrazoles) and 30 other structures, including all possible bis(amino)-azobis(azoles) with an N−N=N−N unit, were designed. The molecular geometries were fully optimized at the DFT-B3LYP level with the 6-31++g (d, p) basis set. From the absence of any imaginary frequency in the infrared vibration frequency spectrum, it is predicted that all these studied structures may exist in stable forms. The results of the total energies of the stereoisomers of 5,5'-bis(amino)-1,1'-azobis(tetrazoles) indicate that the two symmetric trans-form structures are more likely to exist than the other four. The pyrolysis process, chemical stability and molecular electrostatic potential were studied via the investigation of their electronic structure. Heats of formation (HOFs) were calculated using the atomization energy method based on the results of the harmonic vibration frequencies, and a linear relationship was found between the HOF and nitrogen chain or nitrogen content. Densities of the title compounds were predicted with the Monte Carlo method. Finally, according to the results of the calculated HOFs and densities, the explosive parameters of these compounds were calculated using the Kamlet−Jacobs formula. 5,5'-Bis(amino)-1,1'-azobis(tetrazoles) and its isomer 5,5'-bis(amino)-2,2'-azobis(tetrazoles) may have potential for use as energetic compounds.

Extractive-spectrophotometric determination of NTO and TNT in mixtures

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Keywords: Spectrophotometry; NTO; TNT.

An extractive-spectrophotometric method was developed for explosive mixtures where NTO is added as desensitizer to the sensitive TNT. NTO is quantified with the aid of the 416-nm absorbance of its yellow-colored 2Na+NTO2− salt formed with moderate strength aqueous NaOH solution. TNT, if present, is pre-extracted into IBMK as its Meisenheimer anion forming an ion-pair with the cationic surfactant cetyl pyridinium (CP+) in alkaline medium, whereas the unextracted (double negatively-charged) NTO anion is determined in the aqueous phase. The method was shown not to be affected by nitramines (RDX and HMX) and nitrate esters (PETN), tested in either synthetic explosive mixtures or composite explosives (CompB and Octol). The developed methods were statistically validated against HPLC.

Modeling the gas phase partial oxidations of hydrocarbons at moderate temperatures and increased pressure

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Keywords: kinetic scheme; hydrocarbons; oxidation; ignition; critical condition; selectivity.

The detailed kinetic S1-S2 scheme suitable for the description of oxidation of hydrocarbons in a wide range of pressure and temperatures (P=1-100 atm, T=500-1500K) is considered. Feature of model is presence of the block of reactions of so-called peroxide cycle, without which account the correct description the oxidation stages at low temperatures is impossible. During calculations it is shown that the model well reproduces the cores known effects from experiments: delays of Melvin, inhibiting effect of oxygen and promoting effect of pressure, critical conditions of chain and thermal ignition. For the first time the effect of increase of selectivity of oxidizing conversion of superrich metan-air mixes at low temperatures and high pressures is found out.

S,S'-Dimethyl-N-nitroimidodithiocarbonate - precursor of new energetic nitrimines, simple method of synthesis and characterization

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Keywords: dimethyl-N-nitroimidodithiocarbonate; nitrimines.

The S,S'-dimethyl-N-nitroimidodithiocarbonate contains two easy-to-change methylthio groups and therefore will be interest as a precursor of new energetic nitrimines. A simple method has been used to obtain of dimethyl-N-nitroimidodithiocarbonate. UV-, FTIR- and 1H, 13C, 15N NMR-spectroscopy are used to characterize the compound obtained. The degenerate rearrangement in a solution has been discovered.

The crystal and molecular structure of 1-phenyl-2-nitroguanidine

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Keywords: nitrimines; nitroguanidine; x-ray analysis; molecular structure.

The molecule of 1-phenyl-2-nitroguanidine is non-planar but contains two nearly planar fragments – nitroguanyl and phenyl groups. In spite of opposite orientation of a nitrogroup with respect to a substituent in a nitroguanile group, the structure parameters of the last-named group are closely approximated from the parameters of nitroguanidine and its alkylderivatives. An intermolecular interaction results in the violation of the benzole cycle symmetry.

Disposal of explosive ordnance: removal of cadmium from wastewater using modified multi-wall carbon nanotubes

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Keywords: disposal of explosive ordnance; toxic waste; cadmium adsorption; carbon nanotubes; PEG-functionalization.

The use of thermal techniques for disposal of explosive ordnance (EO) generates various toxic substances that pose environmental risks. Such substances, among others, are toxic metals and metalloids. Cadmium, as one of them, is one of the most toxic metals found in the waste. The main goal of this investigation was to reduce the quantity of cadmium below the maximum contaminant level of 0.005 mg dm-3 in wastewater after disposal of explosive ordnance. For that purpose, multi-wall carbon nanotubes (MWCNTs) were functionalized with 6-arm amino polyethylene glycol (PEG) and used for treatment of wastewater contaminated with various concentrations of cadmium at different pH values. PEG-MWCNTs showed best adsorption of cadmium at the pH range 6-8 displaying that there is no need of large increase in wastewater alkalinity during the removal process. The percentage of cadmium removal is above 93% for all studied concentrations of adsorbate.

High-nitrogen heteroaromatics: Relationship between heat of formation and molecular electrostatic potential

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Keywords: high-nitrogen compounds; azines; azoles; heat of formation; molecular surface electrostatic potential.

High-nitrogen heteroaromatics: Relationship between heat of formation and molecular electrostatic potential Monika Bartošková, Zdeněk Friedl Brno University of Technology, Brno, CZ xcbartoskovam@fch.vutbr.cz, friedl@fch.vutbr.cz

ABSTRACT

To characterize explosive properties of high-nitrogen energetic compounds the heats of formation, either in the gas or solid state, are mostly used. Their relationship with the number of nitrogen atoms involved is common knowledge and can not add any new information. On the other hand the very promising QSPR approach utilizes the molecular surface electrostatic potential V(r). In this work we calculated by DFT B3PW91/cc-pVTZ method 11 azines and 9 azoles, respectively, and constructed their gas phase heats of formation Δf H°(298,g) by means of isodesmic reaction approach. Alternatively, we have compared previous values with data obtained from thermochemical G recipes. Acquired gas phase Δf H°(298,g) were correlated with molecular surface electrostatic potentials VS,max , VS,min and VS,Σ which were calculated by B3LYP/6-31G(d,p) method. It is shown that the VS(ring) electrostatic potentials describe most precisely the respective structures of high-nitrogen cumulated heteroaromatics and their thermodynamic properties as well.

Calorimetric correlation of the structure of an energetic polyphosphazene with its heat of formation

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Keywords: bomb calorimetry; energetic polyphosphazenes.

Energetic polyphosphazenes represent a novel class of insensitive binders which out perform conventional carbon-based systems in terms of energy-density and glass transition temperature. Such alternative binders may facilitate the use of more environmentally friendly oxidants such as ADN. For all energetic materials the acquisition of thermochemical data is a necessary prerequisite to performance calculations. We therefore report here on the use of bomb calorimetry to determine the standard enthalpies of combustion (ΔcH^o) and formation (ΔfH^o) of 2,2,2-trifluoroethan-1-oxy/3,4-dinitratopropan-1-oxy polyphosphazene (I) as the proportion of (energetic) 3,4-dinitratopropan-1-oxy substituents (%ES) is varied between 31% and 78%. Similar data is also described for the parent polymer bis(2,2,2-trifluoroethan-1-oxy)polyphosphazene (II) (%ES = 0). ΔcH^o was found to vary between -2275kJmol-1 for the parent polymer II (%ES = 0) and -3415kJmol-1 for I with %ES = 78. The corresponding values for ΔfH^o were -3184kJmol-1 and -1566kJmol-1. It has been concluded from these data that the energetic properties of formulations containing I are likely to be enhanced as the %ES increases, irrespective of whether or not an external oxidant is incorporated into the formulation.

Study of the ignition properties of oriented strand boards exposed to radiant heat flux

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Keywords: ignition; ignition temperature; time to ignition; mass loss.

The paper deals with the study of effect of heat flux on the ignition OSB boards of different thicknesses. Ignition is the first of the fire properties to be taken into account for assessing the fire hazard. Ignition of the materials is contained in ISO standard 5657: 1997, where is described a method for testing the ignitability of building products. It is a simple aspect of the fire situation characterized by a radiant heat source, which are exposed to test samples. It is a modification of this method was used to determine the time to ignition and tested mass loss OSB when exposed to the pre-defined heat flux. Another characteristic observed in this work, the behavior of the plate materials according to the thickness in order to define the behavior of the thermally thin and thermally thick materials exposed to heat flux.

A novel HPLC method for analysis of composite explosives containing NTO and TNT

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Keywords: HPLC; NTO; TNT.

The known composite explosives containing NTO and TNT include 50% NTO–50% TNT known as TNTO, 65% NTO–35% TNT known as GD-1, and 40% NTO–60% TNT known as South African 1. A new HPLC method was developed for the separation and quantification of NTO and TNT. For this purpose, a Hypercarb column having 100% porous graphitic carbon (PGC) spherical particles was used as the stationary phase with gradient elution. The developed low-cost method can be used for rapid and practical analysis of such composites during their whole shelf-life for differentiating between undegraded sensitive and insensitive components; thus, the kinetic stability of munitions containing desensitized energetic materials can be better modeled.

Numerical simulations for prediction of aerodynamic drag on high velocity fragments from naturally fragmenting high explosive warheads

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Keywords: numerical simulation; fragment; drag coefficient.

Numerical simulation of airflow around several representative high velocity fragments, originating from naturally fragmenting high explosive warhead 130mm M79, was performed using FLUENT® finite element method package. FLUENT software contains the broad physical modeling capabilities needed to model flow, turbulence, heat transfer for different applications, ranging from air flow over an aerodynamic surfaces to real combustion processes. Aerodynamic drag coefficients of fragments were predicted for a wide range of Mach numbers and for eight different positions of fragments. Different positions simulate dynamic instability of fragments during their flight through the atmosphere and account for stochastic behavior of fragments, which directly influences aerodynamic drag coefficients and subsequently fragments range and warhead lethal zones. Obtained results of aerodynamic drag coefficients were compared with available experimental data.

Passivated tetrazene for use in small-scale impact-sensitive gas generators

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Keywords: tetrazene; gas generators; green energetics; low-velocity projectiles.

Small-scale gas generators find use in propulsion of low-mass projectiles at typically sub-sonic velocities; one such example is training ammunition. Small-scale gas generators should be compact, reliable, predictably ignitable, and non-toxic. Traditionally, primary explosives, or pyrotechnic mixtures, that contain heavy metals (e.g. lead) provide a means of generating heat and gas reliably, but with the drawback of toxicity. Many new primary explosives have been engineered to address the problems of toxicity, but can be expensive and difficult to synthesise. Tetrazene (1-(5-tetrazolyl)-3-guanyltetrazene) has been widely used as an ignition enhancer in percussion primers for almost a century, but its use as a gas generator is less prevalent. Its high nitrogen content and impact sensitivity make it an ideal impact-sensitive gas generator. This paper presents the use of tetrazene, passivated with paraffin wax, as a reliable, heavy-metal-free and inexpensive alternative to tradi-tional impact-sensitive gas generators. Experimental data showing the tetrazene/paraffin mixture's reliable generation of high-pressure gas from a compact casing are presented. The packaged composition is shown to function in a 9 mm training ammunition system, providing 2.7 g projectiles with mean and standard deviation muzzle velocities of 106 m/s and 5 m/s respectively. The tetrazene/paraffin system shows a significant improvement in repeatability and non-toxicity over the current lead styphnate based system.

Calibration method for velocity of detonation measuring device

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Keywords: explosive materials testing; calibration; velocity of detonation; electro-optical method.

The velocity of detonation is one of basic parameters for determination of explosive power and quality that can be measured. Delay period is of the same importance for detonators and other initiation devices. Determination of those parameters is mainly performed by optical-electrical method by time interval measurement. In Laboratory for testing of explosive material, a method was developed for the calibration of electronic timer with photodiodes and digital oscilloscope. Calibration of electronic timer, velocity of detonation measuring device, is carried out by parallel measuring of a time interval by a digital oscilloscope. Paper describes the setup and measurement conditions, type of instrumentation and accessories of comparison calibration method with review according to the measuring uncertainty and method suitability.

Range of fragments from accidental explosions

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Keywords: sympathetic explosion; explosives; range of fragments.

A possible method for determining initial velocity and range for flying fragments is pro-posed. Quantity-Distance principles are discussed and some arguments are presented for why even the observance of Q-D principles could not prevent sympathetic detonation due to flying fragments. The proposed procedure is based on the principles of explosive load-ing of objects. Example calculations were carried out and the results compared with data obtained from an accidental civil explosion. The results show that this method should be suitable for evaluating fragment velocity and range. Limitations of the method and pro-posals for possible future improvements are discussed in the conclusions.

Sensitivity to Impact of Mixtures Ammonium Perchlorate with Teflon

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Keywords: sensitivity to impact; ammonium perchlorate; teflon.

By means of the method of critical energies the sensitivity indicators to impact for mixes ultradispersed ammonium perchlorate with teflon are defined at various ratios between components. By extrapolation of the received dependences to a limit of the content of pure teflon the crude estimations of top level of force actions, safe for the mechanical handling with teflon are received.

Application of nitrocellulose and cellulose composition in a model reactive armor

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Keywords: nitrocellulose-cellulose composites; reactive armor; Gurney energy.

Monolithic nitrocellulose and cellulose composites (NC-C) were obtained by cross-linking a mixture of nitrocellulose with cellulose using hexamethylene diisocyanate (HDI). They were used in a model reactive armor. The influence of cellulose content on the acceleration ability of the gaseous reaction products of composites was examined by the use of X-ray technique. The modified Gurney model was used to simulate the process of driving steel plates in the reactive armor after jet impact. Formulas for determining the time-space characteristics of movement of the plates were derived. The model was verified by using the results of X-ray recording of plates driven by explosion products of monolithic nitrocellulose and cellulose composites (NC-C).

Simultaneous spectrophotometric determination of HNS and TNT by derivative spectroscopy

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Keywords: HNS; TNT; Derivative Spectroscopy.

As there are no molecular spectroscopic determination methods for the most widely used heat-resistant insensitive explosive 2,2',4,4',6,6'-hexanitrostilbene (HNS) in the presence of sensitive nitro-explosives (e.g., structurally analogic TNT), a novel spectrophotometric method was developed for HNS and TNT assay in mixtures and composites. For HNS and TNT mixtures, both analytes react with dicyclohexylamine (DCHA) forming different colored charge-transfer complexes, which can be resolved by derivative spectroscopy. This method was not affected from nitramines and nitrate esters in synthetic mixtures or composite explosives, and was statistically validated against HPLC.

Investigation on the effect of microencapsulation with some organic coating agents on surface morphology and thermal property of magnesium particles

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Keywords: microencapsulation; magnesium.

Powdered magnesium has a wide range of applications in various chemical, military, pharmaceutical, metallurgical, and agricultural industries. Specific applications include pyrotechnics, steel desulphurization, metal matrix composite fillers and powder metallurgy. Magnesium is a highly energetic material, i.e., it has a tendency to catch fire, especially in pyrotechnics industries. Magnesium powder is one of the most important components of many pyrotechnic explosives because of its good burning and illuminating properties. However, magnesium is very active, and it also has a high affinity with oxygen, nitrogen and water. The formation of magnesium compounds deteriorates many of the desirable properties of ground magnesium, e.g., the reduction or even elimination of its pyrotechnic properties and hence severely limits its applications. In this research, microencapsulation technique based on a solvent/non-solvent method has been used to enhance the oxidation resistance of magnesium powder with nitrocellulose and Viton as alternative coating agents. The coating quality and the mechanism of the nitration/oxidation reactions of pure and coated samples were studied by means of scanning electron microscopy (SEM), thermogravimetry analysis (TGA) and X-ray diffraction (XRD) methods. Thermogravimetry analysis (TGA) of pure sample exhibited two successive phenomenons in the wide range of temperature (at about 500-1200 °C) which related to nitration and oxidation processes respectively. However because of greater thermodynamic stability, at elevated temperatures, any nitride formed is eventually converted to the corresponding magnesium oxide (MgO) compound. Also, these results confirm by XRD and SEM data of Mg particles that heated at different atmosphere and temperatures. Finally, the results of this investigation showed that Mg microparticle could be effectively coated with Viton through a solvent/non-solvent experiment at optimum conditions in which the oxidation reaction occurs at 20°C higher than that of the uncoated particles and overall nitration/oxidation reaction completed under 1000 °C, with 66% mass gain. The result confirms that by coating of Mg particles by proper coating agents, the efficiency of the magnesium based pyrotechnic system can be increased.

Optical absorption spectroscopy investigation on the interaction of tetra (methyl pyridinum -4-yl) porphyrin (TMPyP) and its copper(II) complex (CuTMPyP) with TNT in acetonitrile

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Keywords: cationic porphyrins; 2,4,6- trinitrotoluene (TNT); UV-VIS; thermodynamic parameters.

Interaction of two cationic porphyrins, 5, 10, 15, 20-tetra (Methyl pyridinum -4-yl) Porphyrin (TMPyP) and its Cu (II) complex (CuTMPyP), with TNT in acetonitrile has been studied by UV-Vis spectroscopy. Analysis of the spectral data revealed formation of a 1:1 conjugate between cationic porphyrins and TNT. The binding constants (K11) of this conjugation have been obtained at various temperatures through evaluation of absorption data. The binding constants of TNT to TMPyP and CuTMPyP were decreased with increasing temperature in acetonitrile. The thermodynamic parameters of the process, including entropy and enthalpy changes, have been calculated by means of van't Hoff plots method. The results showed that the TNT binding process for both porphyrins is an enthalpy driven phenomenon.

Preparation and Characterization of 5-Azido-3-nitro-1H-1,2,4-triazole

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Keywords: energetic materials; triazoles; azides; sensitivities; crystal structures.

5-Azido-3-nitro-1H-1,2,4-triazole was synthesized by diazotation of 3-amino-5-nitro-1H-1,2,4-triazole with sodium nitrite and subsequent reaction with sodium azide in aqueous solution. It was fully characterized by vibrational (IR, Raman) and NMR (1H, 13C, 14N, 15N) spectroscopy, mass spectrometry and single crystal X-ray diffraction. Its thermal behavior was analyzed by DSC, the sensitivities were determined according to BAM standards and the performance was calculated with EXPLO5.

Application of pressurized fluid extraction for quantification of propellant components

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Keywords: propellant; analyses; pressurized fluid extraction; gas chromatography/mass spectrometry; GC/MS.

Analysis of explosives, mainly smokeless powders and explosives mixtures, is an integral part of the production of explosives, fulminating compounds or propellants. Nowadays, chromatographic methods are used for these analyses, for example high performance liquid chromatography with ultraviolet detection (HPLC/UV). Modern methods and classical methods of propellant analysis (titration, gravimetry) require sample preparation to analysis. It means that target analytes have to be isolated from sample for their analysis. Isolation step of propellant analysis includes extraction methods usually. The extraction method is always selected according to the matrix of a sample and kind of a sample. Conventional method for preparation of propellant samples and explosives samples is Soxhlet extraction with dichloromethane or diethyl ether as extraction agent. Substitution of Soxhlet extraction and development of new chromatographic method for analyzing of propellant components were major goals of our work. Pressurized fluid extraction (PFE) is modern and efficient extraction method. The same efficiency or higher extraction efficiency using PFE was observed than using Soxhlet extraction (SE). Time of extraction was shorter using PFE than using Soxhlet extraction (8 hours). Combination of gas chromatography and mass spectrometry (GC/MS) is faster, more sensitive and more accurate method for analyses of propellant components than conventional HPLC/UV. First of all, advantage of GC/MS method is detection of newly tested propellant components, because some of them do not provide of response using ultraviolet detector (for example acetyl tributhyl citrate – gelifying agent in propellants). Secondly, substances can be immediately identified by comparing measured MS spectra with library spectra. Therefore, the GC/MS method fulfills also the qualitative part of smokeless powder analysis (especially the unknown ones).

Reduction of quantity of HE in explosive light sources for photorecording schemes

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Keywords: explosive light source; high-speed photographing; burning; fine metal powder.

Argon glow lamps are traditionally used at carrying out the high-speed photographing with characteristic time of shooting from 0.5 to 10 ms. Thus, large mass charges of explo-sives (10 kg and more) are applied. Such practice cannot be approved. It is dangerous to the personnel and the equipment participating in experiment. The given method harms the nature: strong air shock, soiled environment with explosion products. Some results on light source development are presented. The principle of explosive ignition of a fine metal pow-der is applied. It is suitable for typical schemes of high-speed photographing, and, at the same time, contains small quantity of explosive (less then 30 g).

The correlation relations between the secondary explosives' deflagration temperatures and their 5-second delay burst temperature

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Keywords: secondary explosives; burst temperature; DTA; deflagration beginning temperature; maximum temperature of deflagration; correlation.

The values of deflagration beginning temperature and maximum temperature of deflagration (Tdb, Tmax) for 24 secondary explosives of different classes are obtained using DTA method. The linear correlations between Tdb and Tmax were found. The linear correlations between the 5-second delay burst temperature (Tburst(5s)) and Tdb, Tburst(5s) and Tmax were found.

The reaction of trinitromethylation-diaroxylation of 2,4,6-trichloro-1,3,5-triazine

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Keywords: Trinitromethane salts; 2,4,6-trichloro-1,3,5-triazine; phenols; reaction of trinitromethylation-diaroxylation.

The interaction of 2,4,6-trichloro-1,3,5-triazine with trinitromethane salts in presence of phenol and substituted phenols was studied. It was shown that the interaction goes along with the reaction of trinitromethylation-diaroxylation of 2,4,6-trichloro-1,3,5-triazine which leads to the formation of the appropriate 2,4-diaryloxy-6-trinitromethyl-1,3,5-triazines.

Optical initiation of energetic materials. Recent scientific investigations and technical applications

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Keywords: energetic material; optical initiation; laser detonator; initiation system.

Research on the use of a light pulse for initiation of primary explosives began in the 50-th years of the past century. However, consecutive expansion and deepening of work in this direction began only in the 60-th years since the advent of laser light sources. Intensity of such research was conditioned by the fact that the method of optical initiation of explosives has a lot of advantages in comparison with the methods of electrical initiation. These advantages are the heightened safety of laser initiation systems to the extraneous sources of electric and electromagnetic signals, the opportunity of using less sensitive explosives and pyrotechnic compositions in initiators and igniters, and the greater potentialities of employing the method in complex technical systems. By now a great many research papers concerned both with studying the processes of initiation and ignition of various energetic materials and with developing the various technical and military applications of these phenomena have been published. The presented overview enables everyone to familiarize oneself quickly with the situation existing in this field of research for about the semicentennial period of its progress, to estimate possibilities for further investigations in this direction, and to plan ways of adoption and utilization of the results obtained by this time. The following basic problems have been considered and presented in the overview: the initiation of traditional primary explosives; the initiation of secondary high-energy explosives; the initiation of explosives on the basis of coordination compounds; the initiation of pyrotechnical compositions; the ignition of pyrotechnical compositions, smokeless powders, rocket propellants and secondary explosives; the surface initiation of explosive layers; the development of optical laser detonators; the creation of optical initiation systems. The basic factors associated both with the properties of energetic materials and with the characteristics of irradiating pulse have been revealed, some physical models of initiation have been created, a whole class of laser detonators and initiation systems has been developed by now. Some concrete technical applications have been also discussed in the overview.

Synthesis and fluorescence quenching studies on a quinoline derivative in the presence of TNT

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Keywords: 2-phenylquinoline-4-formic-acrylic-diol-diester(PQFAED); explosives detection; fluorescence quenching; TNT.

A novel fluorescent compound 2-phenylquinoline-4-formic-acrylic-ethylene glycol diester (PQFAED) was synthesized by the esterification reaction of 2-phenylquinoline-4-carboxylic acid and 2-Hydroxyethyl acrylate. Its structure were characterized by FTIR, 1HNMR and EA. The absorption spectra and fluorescence spectra of PQFAED have been obtained. Fluorescence analysis technique was used to research fluorescence response of the PQFAED to trace nitro-explosive (TNT) in practice. The test results showed that when fluorescent compound of PQFAED interacting with TNT, the fluorescence intensity goes on decreasing with the concentration of TNT increasing in this system. Therefore, PQFAED has potential application in nitro-explosives detection.

Thermoanalytical investigation on some ammonium azide binary pyrotechnic mixture as novel chemical gas generating systems

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Keywords: gas generation ; ammonium azide ; pyrotechnic mixture.

Pyrotechnic compositions are typically composed of finely divided mixtures of metallic or non-metallic elements as reducing agent with some oxidizing agents to chemically generate gas, heat, light, or color and used in air bag inflators, smoke dye, emergency signaling, fireworks, and special effects devices for the entertainment industry. Previous studies revealed that sodium azide was used in several mixtures as a main component for gas-generation process. Also, sodium azide constitutes major fraction of several pyrotechnic mixtures in which plenty of pure nitrogen gases and a sodium aerosol release upon their high temperatures combustion. The conventional NaN3/oxidants gas generator pyrotechnic mixtures suffer from toxic problem and a lot of solid residues. The aim of present investigation is to overcome this disadvantage by combination of NH4N3 particles with some metallic component and introduces novel gas generator pyrotechnic mixtures. In this work, primarily according to our recent investigation, volatile ammonium azide particles stabilized via its microencapsulation technique, and then, the NH4N3/reducting agent's compositions with Zr, Ti, ZrH2 and TiH2 powders as a different reluctant agents were prepared. Subsequently, the thermal properties and kinetic parameters of these pyrotechnic mixtures were investigated by using thermal analysis (TG/DTA and TG) techniques. Also, the apparent activation energy (E), ΔG#, ΔH#, ΔS# and Critical ignition temperature (Tb) of the ignition processes of mixtures were obtained from the DSC experiments. Finally, among the investigated mixtures, NH4N3/TiH2 composition has been found to show desirable gas generating efficiency and can be considered as a safe and efficient pyrotechnic composition for gas generation property, due to its moderate safe ignition temperature.

Theoretical Studies on Mononitro, Dinitro, and Trinitro Derivatives of 1-Aminoimidazole

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Agency for Defense Development

Keywords: aminoimidazole; molecular structure; explosive property; impact sensitivity.

Molecular structures and chemical properties of mononitro, dinitro, and trinitro derivatives of 1-aminoimidazole have been investigated at high levels of density functional theories. Heat of formation, density, explosive performances and impact sensitivities have been estimated at the global minimum of potential energy surface by following the scheme developed by Cho (ref. Cho, A Systematic Procedure to Predict Explosive Performance and Sensitivity of Novel High-Energy Molecules in ADD, ADD Method-1, In Handbook of Material Science Research, Charles René and Eugene Turcotte, Eds., Nova Science Publishers, Inc., New York, 2010, Chapter 11.). As more nitro groups are introduced, the explosive performances of 1-aminoimidazole derivatives are enhanced, while the impact sensitivity becomes more sensitive. According to our two-dimensional plot between explosive performance and impact sensitivity, 1-aminodinitroimidzole isomers appears to have a potential to be good candidates for insensitive explosives, and 1-aminotrinitroimidazole may become a powerful explosive molecule whose behavior is quite close to HMX.

A Virtual 3-D Chemical Database for High Energy Molecules in South Korea: MS-HEMs

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Keywords: virtual database; high energy molecule; search; screening; molecular descriptor.

A pioneering version of an on-line management system for high-energy molecules (MS-HEMs) was developed by the ADD and BMDRC in South Korea. The current system can manage the physicochemical and explosive properties of virtual and existing HEMs. The on-line MS-HEMs consist of three main routines: management, calculation, and search. The management routine contains a user-friendly interface to store and manage molecular structures and other properties of the new HEMs. The calculation routine automatically calculates a number of compositional and topological molecular descriptors when a new HEM is stored in the MS-HEMs. Physical properties, such as the heat of formation and density, can also be calculated using group additivity methods. In addition, the calculation routine for the impact sensitivity can be used to obtain the safety nature of new HEMs. The impact sensitivity was estimated in a knowledge-based manner using in-house neural network code. The search routine enables general users to find a exact HEM and its properties by sketching a 2D chemical structure, or retrieve HEMs and their properties by giving a range of properties. These on-line MS-HEMs are expected be powerful tool for deriving novel promising HEMs.

New Mild Synthetic Schemes for 1,2-Bis(5-nitroiminotetrazol-1-yl)ethane

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Keywords: tetrazole; explosive; nuclephilic substitution; alkylation; nitration.

A novel mild synthetic method to prepare 1,2-bis(5-aminotetrazol-1-yl)ethane (1) was developed from 1-(2-chloroethyl)-5-aminotetrazole (2) and sodium 5-aminotetrazolate (3). The alkylation of 3 was also performed using 1,2-dibromoethane (4) by following the experimental procedure by Barmin et al. (ref. Russ. J. Appl. Chem. 2001, 74, 1156.) and modifying the separation method. Highly energetic compound, 1,2-bis(5-nitroimidotetrazol-1-yl)ethane (5), was synthesized by nitrating 1, which was present as a mixture with 1-(5-aminotetrazoly-1-yl)-2-(5-aminotetrazol-2-yl)ethane (6). Our new synthetic scheme without using highly toxic cyanogen azide may enable to us to produce a large quantity of 5.

Sensitivity of Bis(3(5)-hydrazino-4-amino-1,2,4-triazole) Copper (II) Perchlorate with Additives to Laser Pulse

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Keywords: IR-laser; pulse; ignition; copper complex perchlorate; 3(5)-hydrazino-4-amino-1,2,4-triazole; light-sensitive explosive.

It was shown that the threshold of laser initiation of the copper complex perchlorate with 3(5)-hydrazino-4-amino-1,2,4-triazole as a ligand changed under the influence of additives of an optically transparent polymer, detonation nanodiamonds or carbon nanotubes.

Use of a Hot-Spot Model to describe the influence of particle size and distance between particles on the combustion in a cloud

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Keywords: combustion; particles; hot-spot-model.

The combustion of particles in a cloud can be very different from single particle combustion. In addition to the size of the particles, the number density of particles or the mean distance between the particles plays an important role. Experiments show, if the distance between the particles in a cloud is large enough, particles burn similar to single particles. But below a certain distance particles form a common flame front. In a parameter study a hot-spot model is used to simulate the two burning regimes and to find critical parameters for the transition between them. The results are discussed in the scope of the combustion of metalized gelled and solid propellants and dust explosions.

Energetic Salts of the Azidotetrazolate-2-oxide Anion

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Keywords: tetrazoles; energetic materials; azides.

The highly-sensitive 5-azidotetrazolate anion was oxidized to its corresponding N-oxide by aqueous oxidation in a buffered oxone solution to the azidotetrazolate-2N-oxide anion. After acidic extraction and neutralization with ammonia, the ammonium salt was isolated. Several energetic salts of this novel anion were prepared from the ammonium salt, and in all cases were found to be of lower sensitivity than the corresponding 5-azidotetrazolate salt, while still being highly-sensitive towards mechanical stimuli. Explosive performances (detonation velocity, detonation pressure) of applicable salts were also found to be higher than the non-N-oxide variants. Preparation of the free acid 2-hydroxy-5-azidotetrazole was achieved by protonation of the anion and identified by NMR spectroscopy, where as the majority of the azidotetrazolate-2N-oxide salts have unequivocal crystallographic proof.

Products of transformation of hydroxy-derivatives of N-heterocyclic compounds under conditions of oxidation and nitration

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Keywords: hydroxy-derivative of pyridine; pyrazine; quinoline; oxidation; nitration; crystal structures.

Reactions of oxidation and nitration of hydroxy- and amino-derivatives of pyridine, pyrazine, and quinoline are studied. Depending upon the conditions (temperature and time of heating, catalyst presence, concentrations of oxidizing and nitrating products), a variety of nitro- and oxo-derivatives were isolated with different yields. The major products were characterized by X-ray analysis on single crystals.

Detonation velocity of mixtures based on various dispersed ammonium nitrate

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Keywords: improvised explosive; ammonium nitrate; detonation velocity.

At previous NTREM seminars were reported about the results of investigations of failure detonation diameter of mixtures based on granular and fine-dispersed ammonium nitrate (AN) with different quantities of aluminum powder. In this work were carried out the measurements of detonation velocities of mixtures based on granular AN with content of Al C=1,4%, that, as were shown at previous works, conformed to minimal failure diameter of detonation for that mixture, and mixtures based on fine-dispersed AN with content of Al at zero oxygen balance and contents that most used in improvised explosive devices.

Transformation of metals at explosion at impact of mixtures of them with high explosives

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Keywords: aluminium; condensed products; explosion at impac; temperature of explosion.

It has been shown in previous investigations that all aluminium powder turned into aluminium oxide at explosion at impact of mixtures of it (10%) with typical energetic material such as HMX. On the contrary aluminium oxide was not found at all after explosion of mixture of benzoyl peroxide with aluminium or with aluminium hydride in these conditions. This fact gave an opportunity to conclude that temperature of BP/Al explosion was not more that which has been measured at burning (833 K), i.e. it did not culminate to thermodynamic value. In next work the quantity of explosives – aluminium mixtures under investigation were extended. Peroxides: TATP and HMTD and nitrocompounds of various classes: c-nitrocompounds (TNT, picric acid), nitroethters (PETN, nitrocellulose (NC) with content of nitrogen CN=11.6%), compound that was at the same time c-nitrocompound and N-nitrocompound (Tetryl) were used as explosive base of mixtures. It was found practically all aluminum or aluminum hydride in mixture of it with explosive (Picric acid, HMTD, NC, Tetryl, PETN, HMX) transforms into aluminum oxide if calculated temperature of explosion of a mixture Tpş2200 – 2300 K. In this work the data of analysis of condensed products of explosion and calculated temperature of explosion of mixtures high explosives with alloy of Mg and Al were carried out and compared with previous results. The main condensed product (98%) at explosion at impact in this case was spinel Mg(AlO2)2.

Thermal decomposition of the geminal dinitroethylmethylnitramines

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Keywords: kinetics; thermal stability; gem-dinitroethylmethylnitramines; mechanism; steric effect.

The influence of nature of a-substituent at geminal dinitrogroup upon the thermal stability of secondary methylnitramines is studied. The limiting stage of thermal decomposition is established and its activation parameters are determined. The steric effect of substituent renders the essential influence upon the thermal stability of geminal dinitrogroup in nitramines together with an induction and resonance component. Between the rate constant, activation energy and the steric constant Es the correlation dependence is found, which has a prognostic ability.

Safe design of flashbang

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Keywords: non-lethal weapon; blinding means; gas-dynamic drive; photo mixture.

Devices with pyrotechnic generation of light and acoustic impulses (flashbang) are ap-plied, as special police means for suppression of criminals. Another approach is shown in this paper. The charge of explosive of small weight (no more than 15 g) is used in the scheme with gas-dynamic driver that simultaneously rises safety up. Test results are pre-sented, they confirm working capacity and non-lethal applications of the prototype of the new explosive flashbang.

Characteristic analysis of tungsten type delay composition during thermal aging

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Keywords: thermal aging; tungsten type delay composition; delay time; thermal conductivity; aging mechanism.

Change in the performance parameters of tungsten type delay composition with thermal aging time and aging mechanism were discussed in this paper. The main research contents include: effects of granulation on delay time and thermal conductivity; influence of tungsten content on delay time and thermal conductivity; the change law of delay time and thermal conductivity with thermal aging time; study on influence of thermal aging on thermal decomposition characteristics. Results show that: (1) during thermal aging, the delay time of tungsten type delay composition drift. The higher the quantity of the tungsten, the lager the delay time drift and the more difficulty the delay time to get steady; (2) the delay time of reagent without granulation just has little change and reaches stable faster than the reagent with granulation of the same formula; (3) thermal conductivity increases with the storage time, the higher the quantity of W content, the faster the thermal conductivity changed, and granulation delays the aging of tungsten type delay composition. (4) Tungsten type delay composition decomposes at temperatures between 379.8 600°C and the pre-ignition reaction zone moves toward higher temperature and need more energy after stored at elevated temperatures. (5) The aging mechanism of tungsten type delay composition is a solid state reaction. That is, the reducing agent tungsten reacts with the oxidant potassium perchlorate and formed tungsten oxide on the surface, therefore, its activity decreased and delay time lengthened. Based on the thermal aging experiment and decomposition mechanism, method to improve the stability of delay time was put forward in this paper.

Effect of modification of test conditions of zircon composition sensitivity to electrostatic discharge upon test results

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Keywords: high sensitivity EM; electrostatic discharge test; activation.

The paper presents results of methodically outlined tests for determination of zirconium composition sensitivity to energetic effects of electrostatic discharge. These tests are performed at the IEM workplace with the use of a multipurpose apparatus ESZ KTTV, which by application of standard methodology allows testing of current EM as well as those being developed. The output data of a test series are always loaded with a certain scattering, which is partly due to slight deviations of the test conditions from the established standard. The results of methodical tests performed within limiting test conditions document the fact that the activation or non-activation of the composition samples also depends upon the diversity of courses of individual tests.

Synthesis of energetic materials in ionic liquids

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Keywords: energetic materials; ionic liquids.

Ionic liquids (ILs) have been widely employed over the past 10-15 years as a potential replacement of conventional solvents and catalysts for a variety of chemical processes. ILs have considerable advantages over available organic solvents – they are fire-resistant and have limited vapor pressure thus allowing efficient recovery of organic products. It was found that many reactions gain acceleration in ILs due to solvatation of forming charged intermediates or ions. In many cases ILs display a catalytic activity. In addition, ILs are recyclable and can be reused several times in the same reactions. The realization of different reactions in ILs pertains to a new prospective field of organic chemistry – "green chemistry". We have found that ILs also are an excellent reaction medium for the very diverse organic reactions leading to energetic materials. These investigations allowed developing ecologically pure methods for the preparation of both known and new EMs, containing heterocyclic fragment (furazans, furoxans, tetrazoles), as well as structures with high content of oxygen (e.g. trinitroethyl derivatives). In contrast to known methods reactions in ILs are carried out without heating, that provide for safety of processes and as rule the target products are formed with more high yields and purity, and ILs being not only reaction medium but and catalysts, can be regenerated and reused several times in the same reactions.

Study of Ageing Processes of Double Base Rocket Propellants, Based on Stabilizer Consumption

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Keywords: activation energy; artificial ageing; double-base propellant; kinetics of decomposition; ethyl-centralite; liquid chromatography (HPLC).

The aging of double base (DB) rocket propellants is the result of chemical decomposition reaction and physical processes, causing degradation of a number of relevant propellant properties (such as reduction of stabilizer and nitroglycerine (NG) content, reduction of mean molecular mass of nitrocellulose (NC) etc.), which reflects on the reduction of reliable application time of DB propellants. In certain circumstances, the processes of chemical decomposition can take autocatalytic character and lead to the well-known phenomenon of "self-ignition or thermal explosion" of propellant. Consequently, studying of the mechanism and kinetics of the processes that cause propellant aging has great practical and theoretical importance. In order to investigate the aging process of DB rocket propellants, propellant samples were subjected to accelerated aging at elevated temperatures (80, 85 and 90 °C), and the change of the stabilizer/ethyl-centralite content with aging time and temperature were periodically monitored. Change of the ethyl-centralite content was observed using liquid chromatography (HPLC). The results show that ethyl-centralite consumption in conditions of accelerated aging is very intense from the very beginning of aging. The entire ethyl-centralite is depleting after 120 days at 80 °C, followed by the intensive reactions of NC decomposition. The results obtained from kinetic data processing have shown that activation energy of DB propellant decomposition obtained on the basis of ethyl-centralite consumption is 142.98 kJ/mol, which is consistent with available literature values.

Study about the amount of air cooling of j85-21GE engine's shell untill it reaches a desirable temperature

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Keywords: combustion chamber ; shell; PDF model; flow; cooling.

Abstract The main emphasis in this paper is to account required flow quantity of air cooling of circular combustion chamber of shell which is a part of j85-21GE engine's shell. Our purpose is to reach a desirable temperature for example 100 C by modeling three-dimensional combustion in a 30 cut. The amount of heat transfer and temperature changes become distinct on the outer shell. We reach a desirable temperature from shell's temperature by creating a flow field around shell and injecting flow (cold air) into two standard situations of surface with speed of 0.9 mach and into a height of 33000ft with speed of 1.6 mach. The result have analyzed by encoding a computerized program using empirical relations. It follows good result of numerical analyses. The used turbulent model is Realizable and it's combustion model is modellized by probability density function(P.D.F).

Study of metal salts of the 4,5-dicyano-2H-1,2,3-triazole anion as pyrotechnic ingredients

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Keywords: triazoles; energetic salts; X-ray crystallography.

Diaminomaleodinitrile was reacted at low temperatures with in situ generated nitrous acid to form 4,5-dicyano-2H-1,2,3-triazole (1) in yields above 90 %. Crystalline 1 was then re-acted with one equivalent of a suitable alkali or alkaline earth metal base (typically a hy-droxide or a carbonate) in a polar solvent to form the corresponding alkali and alkaline earth metal salts of 4,5-dicyano-2H-1,2,3-triazole (compounds 2–9). The thermal stability of the metal salts 2–9 was assessed by differential scanning calorimetry, which showed ex-cellent thermal stabilities up to above 350 °C. Due to the energetic character of triazole-based salts, initial safety testing was used to assess the sensitivity of compounds 2–9 to-wards impact, friction, electrostatic discharge and fast heating. These results revealed very low sensitivities towards all four stimuli. Additionally, compounds 2–9 were charac-terized by mass spectrometry, elemental analysis, infrared and Raman spectroscopy and (1H, 13C and 14N) NMR spectroscopy. We also determined the solid state structure of the 4,5-dicyano-2H-1,2,3-triazole anion of one of the alkali metal salts (4: Monoclinic, P21/c, a = 9.389(1) Å, b = 10.603(1) Å, c = 6.924(1) Å, β = 102.75(1)° and V = 1036.58(3) Å3) and one of the alkaline earth metal salts (6: Monoclinic, P21/c, a = 9.243(1) Å, b = 15.828(2) Å, c = 6.463(1) Å, β = 90.23(1)° and V = 945.5(2) Å3). Furthermore, we noted the hydrolysis of one of the cyano groups of the 4,5-dicyano-2H-1,2,3-triazole anion in the strontium salt 8 to form the 5-cyano-2H-1,2,3-triazole-4-carboxylic acid derivative 8b, as confirmed by X-ray studies (8b: Monoclinic, P21/n, a = 6.950(1) Å, b = 17.769(1) Å, c = 13.858(1) Å, β = 92.98(1)° and V = 1709.1(1) Å3). Lastly, we computed the NBO and Mül-liken charges for the anion of compounds 2–9 and those of the anion of compound 8b.

Quaternary Ammonium Energetic Salts

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Keywords: ammonium salts; hydrazines; energetic materials; X-ray studies.

1,1-Dimethylhydrazine can be readily alkylated with bromoacetonitrile to form 1-cyanomethyl-1,1-dimethylhydrazinium bromide ([(CH3)2N(CH2CN)NH2]Br, 1). The me-tathesis reaction of compound 1 led to the formation of a new family of energetic salts based on the [(CH3)2N(CH2CN)NH2]+ cation and nitrate (2), perchlorate (3), azide (4), 5-aminotetrazolate ([H2N–CN4]–, 5), 5,5'-azobistetrazolate ([N4C–N=N–CN4]2–, 7) and picrate (8) anions. The new materials were characterized by elemental analysis, mass spectrometry and (multinuclear) NMR and vibrational (infrared and Raman) spectro-scopies. Additionally, the molecular structure of the [(CH3)2N(CH2CN)NH2]+ cation in compounds 1, 3 and 8 was solved by X-ray diffraction techniques. The hydrogen-bonding networks found in the structure of salts 1, 3 and 8 are described using graph-set analysis. The melting and decomposition points of the new compounds were determined by differen-tial scanning calorimetry and insight into their sensitivity towards impact, friction and electrostatics was gained by submitting the materials to standard tests. Furthermore, we estimated some performance parameters of interest and we predicted the decomposition gases formed upon decomposition of salts 2, 3, 4, 5, 7 and 8 and that of mixtures with an oxidizer. The interesting thermal, sensitivity and performance properties of some of the compounds described in this work make them attractive towards a prospective energetic application.

Plastic Bonded Explosive Based on PBAN

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Keywords: PBX; IM.

Methods of testing insensitive material (IEM) and results of testing are presented. The aim of work was developing domestic melt cast plastic bonded explosives composition (PBX), based on domestic materials that could be used to fill munitions shell to obtain IM. Keywords: PBX, IM,

A Preliminary Study of Some Factors Causing High Density of Polynitro Compounds

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Keywords: nitro compounds; explosives; electron density; molecular simulations.

Several selected model molecules of polynitro compounds were used for calculation of electron density distribution particularly focused on the oxygen atoms of nitro groups. On the basis of X-ray data, markedly smaller interatomic O...O distances of nitro groups in neighboring molecules were found as compared with the van der Waals radii for oxygen in those cases where a lower partial electron density was (and the therefrom following lower repulsion forces were) calculated at these oxygen atoms. In contrast to that, the presence of hydrogen bonds in the molecule results in a density increase of the substance. Obviously, both these factors result in unusually high density values of polynitro compounds.

The design of high-safety instant-action electric blasting cap

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Keywords: non-primary explosive blasting cap; deflagration-to-detonation transaction; confinement; secondary explosive.

The design of high-safety instant-action non-primary explosive electric blasting cap is offered. The principle of operation of the offered electric blasting cap is based on deflagration-to-detonation transaction of the secondary explosive in the confinement. The efficiency and the operation reliability of the offered electric blasting cap is shown.

Synthesis and properties of 3-nitroguanidino-1,2,4-triazolo[4.3-b]-s-tetrazine and its salts

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Keywords: triazolotetrazine; synthesis; decomposition; combustion.

The synthesis of 3-nitroguanidino-1,2,4-triazolo[4.3-b]-s-tetrazine (NGuTrTz) and its salts with triaminoguanidine, diaminoguanidine, ammonia, and silver has been carried out in two steps, starting from the readily available 3-(3,5-dimethylpyrazol-1-yl)-1,2,4-triazolo[4.3-b]-s-tetrazine. The nucleophilic substitution of the dimethylpyrazol moiety by nitroguanidine was accomplished in methanol in the presence of sodium methylate. The substitution reaction appeared to proceed rapidly and selectively to yield the sodium salt of NGuTrTz. The sodium salt was isolated and converted to NGuTrTz by treatment with aqueous hydrochloric acid. The other salts of NGuTrTz were obtained by the reaction with aqueous solutions of triaminoguanidinium, diaminoguanidinium, and ammonium hydrochlorides, or silver nitrate. The synthesis of hydrazinium salt was easily performed by reacting NGuTrTz with one equivalent of hydrazine hydrate. The new energetic compounds were identified by FTIR, 1H, 13C NMR spectroscopy, LC-MS and elemental analyses. The thermal decomposition behavior of the new substances was studied by differential scanning calorimetry (DSC). The combustion of some salts of 1,2,4-triazolo[4.3-b]-s-tetrazine was studied in a constant-pressure bomb in the pressure interval of 0.1-10 MPa. The combustion behavior of low-sensitive triaminoguanidinium and hydrazinium salts was compared with that of well-known polynitrogen compound BTATz. The salts demonstrated similar burning rates while having lower pressure exponent.

Some Derivatives of Benzofuroxan (Benzo[1,2-c]1,2,5-oxadiazole N-oxide): Recent Studies on the Synthesis and Properties

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Keywords: benzofuroxan (Benzo[1,2-c]1,2,5-oxadiazole N-oxide); energetic materials; nitrocompounds; synthesis; X-ray diffraction; structure; density; HEDM.

5,6-Dinitrobenzofuroxan (5,6-DNBF) was prepared by 3-step reaction sequence: a) 3-nitrophenylazide was synthesized by diazotation of 3-nitroaniline with sodium nitrite and subsequent reaction with sodium azide in acetic/sulfuric mixed acids solution, b) it was nitrated by HNO3/H2SO4 mixture to 2,4,5-trinitrophenylazide, c) termocyclization of the later compound in the polar solvent medium gave the desired 5,6-DNBF (m.p.177 oC). It was fully characterized by UV/VIS, FT-IR and NMR (1H, 13C) spectroscopy, mass spectrometry and single crystal X-ray diffraction. The density of the resulted compound obtained from its X-ray structure investigation was found as comparatively high value (1,88g/cm3), superior to previously known isomeric energetic material - 4,6-dinitrobenzofuroxan (4,6-DNBF) (1,76 g/cm3). Furthermore the synthesis of some benzofuroxan derivatives, potentially interesting as high-energy and density energetic materials (HEDMs), has been proceeded. Densities of obtained compounds were calculated using ACD Labs software (version 4.0). According to the obtained results it could be concluded that 5,6-DNBF is one of the most dense nitroderivatives of benzofuroxan comparable to CL-14, CL-17, CL-18, so it could find a potential application as HEDM.

Influence of local atmosphere characteristics to range of 155 mm M864 projectile

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Keywords: base bleed; mass flow rate; injection parameter.

Projectiles with base bleed use concept of reducing base drag using injection gas, generated by burning composite propellant into the base area. Influence of atmosphere characteristics at different geographic locations and positions of firing locations, with respect to local conditions, to drag coefficient of 155 mm M864 was analyzed using commercial CFD software FLUENT®. The M864 projectile is chosen because there are many available experimental data. Base bleed output mass flow rate depends on the chamber pressure, the pressure into which it exhausts, time and spin rate. Average injection parameter is estimated using mass of propellant and burning time. Ignition phase of propellant burn is taken into account.

Structure and some properties of the salts of N-nitrozo-N-ethyl(phenyl)hydroxylamine

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Keywords: N-nitroso-N-hydroxylamine; the DFT calculated; enthalpy of detonation; oxygen balance; complex formation.

The electronic structure of potassium salts of N-nitrozo-N-eyhylhydroxylamine (EGA) and N-nitrozo-N-phenylhydroxylamine (PGA) are studied. The enthalpy of formation, combustion and detonation of K(EGA) are calculated by the DFT computational method. It is shown that at 220–240°C the substances explore both in air and in Ar. Spectrophotometric titration of aqueous solutions of ENGA and PGA by the salts of some transitional metals allowed to calculate the composition and formation constants of co-ordinate compounds.

Alternative coating materials for preparation of high temperature resistant PETN or RDX granulates

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Keywords: RDX; PETN; polyurethane; stearates; hydroxystearates.

RDX or PETN phlegmatized with thermo-stable phlegmatizing agent are required by the customers from time to time, to be used for applications in blasting caps or boosters. TNT and waxes are not suitable because of their low melting points. According to our experience, one of suitable coating agents is polyurethane-acrylic copolymer, another one is Zinc 12-hydroxystearate. If compared with zinc stearate, the film of zinc 12-hydroxystearate formed on PETN crystals is more uniform, probably due to polar character of hydroxy group bonded on carbon chain and better adhesiveness to PETN crystal surface. Some sensitivity characteristics of laboratory prepared samples of phlegmatized PETN and RDX were measured and evaluated.

Investigation on the crystal transition of ε-CL-20 in different commonly-used solvent systems

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Keywords: CL-20; crystallization processes; crystal transition; mixed solvents.

The crystal forms of CL-20 obtained from recrystallization of ε-CL-20 in a single or mixed solvent were characterized and confirmed by using Fourier Transform Infrared Spectroscopy (FTIR) and Scanning Electron Microscope (SEM) technique. It was indicated that the ε-CL-20 change its crystal form only when it was recrystallized in single solvent acetone and ethyl acetate. The crystal form of the samples obtained from mixed solvents would transform into α pattern in solvents containing a certain volume of acetone. Particularly, crystal form of ε-CL-20 can stay stable in the mixed solvents containing ethyl acetate.

Producing binder of C4 plastic bonded explosive by a green solvent

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Keywords: C4 plastic bonded explosive; Chlorothene; polyisobutylene; AW-406 solvent.

Chlorothene is toxic and ozone depleting substance which is used as solvent of polyisobutylene in C4 synthesis process. Due to eliminate environmental effects of chlorothene, AW-406 solvent is replaced. The solubility parameter of chlorothene and AW-406 is similar to each other, so polyisobutylene is solved. Polyisobutylene solubility tests are done in two methods: 1) decreasing solvent by evaporation, 2) increasing solvent in weighted ratio. Results of two methods shown that polymer is dissolved well in 1:2 and 1:3 ratios by the least amount of solvent. Dissolved polymer as binder is mixed with plasticizer and RDX. The C4 plastic bonded explosive is made by these two methods is passed standard tests very good.

Thermal Behaviour of Sucrose/Oxidant Binary Pyrotechnic Systems

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Keywords: TG/DTA; thermal stability; organic fuel; pyrotechnic; oxidizer effect; ignition temperature.

Thermogravimetric analysis (TGA) and differential thermal analysis (DTA) have been used to examine the thermal behavior of powdered sucrose with some pyrotechnic oxidants, in relation to the behavior of the individual constituents. The results showed that decomposition temperature for pure compounds (potassium chlorate, potassium perchlorate, potassium nitrate, potassium permanganate, and barium nitrate) are 472, 592, 700, 290, and 745°C, respectively. Pure sucrose powder decomposed in air at about 180°C. On the other hand, TG/DTA of sucrose+KClO3 indicate that this mixture ignites at 183.5°C. Also, when KClO3 is replaced by KClO4 as oxidizer of the fuel, sucrose, the sensitivity of the mixture to thermal ignition will decrease. Sucrose+KNO3 pyrotechnic mixture has ignition temperature around 340°C. Sucrose+KMnO4 pyrotechnic system decomposes at 237.5°C. However, when KMnO4 is replaced by Ba(NO3)2 as oxidizer in pyrotechnic mixture containing sucrose, the ignition temperature increases to 555°C.

Synthesis and studies of new 9-derivatives of polynitrofluorenes

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Keywords: polynitrofluorenes; thermal behaviour; crystal structure; quantum-chemical modelling.

A serie of 9-derivatives of polynitrofluorenes is isolated and studied by the help of a set of physico-chemical methods, i.e. X-ray analysis on single crystals, thermal analysis, quantum-chemical modelling. The crystal, molecular and electronic structure of 2,4,5,7-tetranitro-9-(N-dimethylamino)fluorene are discussed.

Photo-induced decomposition of Energetic Materials

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Keywords: energetic materials; photodecomposition mechanism; experimental conditions.

The photodecomposition mechanism of energetic materials depend on the molecular struc-ture, different photodissociation wavelengths,material's phase, experimental pressure and temperature et al. The photodecomposition mechanisms are not the same by varying the experimental conditions. In this paper, the significant progress on the photodecomposi-tion mechanism of some important energetic materials achieved in recent years are intro-duced in detail, including DMNA (dimethylnitramine), TATB (1,3,5-triamino-2,4,6- trini-trobenzene), RDX (1,35-trinitro-1,3,5-triazacyclohexane), HMX(1,3,5,7-tetranitro-1,3,5,7-tetrazacyclotane) and CL-20 (2,4,6,8,10,12-hexanitro-2,4,6,8,10,12- hexaazaisowurtzi-tane). The difficulty and prospect of the research of the photodecomposition mechanism of energetic materials are also disscussed.

Crystallization of nitroguanidine from different solvents

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Keywords: nitroguanidine; crystallization; spherical crystal.

Nitroguanidine (NQ) is an important low sensitivity explosive widely used as ingredient of propellants. Crude NQ after synthesis and purification in water is in form of long needles which are useless in propellant application. The known methods of controlled crystalliza-tion of nitroguanidine are reviewed. Solubility of NQ in popular solvents like acetone, chloroform, diethyl ether, n- and 2-propanol, carbon tetrachloride etc were studied. Ex-periments were conducted by mixing of non-saturated NQ solution with selected anti-solvent. In typical experiment, solution of NQ in N-methylpyrrolidone was poured into stirred pure cold solvent. Solid precipitate was collected by filtration, dried and weighed. Nitroguanidine crystals with different morphology like rod, needles or spheroidal were successfully produced. The crystallization products were analyzed using 1H, 13C NMR, FTIR spectroscopy, scanning electron microscopy (SEM) and optical microscopy. Bulk density studies for selected samples were conducted.

Comparison of the sensitivity of CL-20 with different phlegmatizers

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Keywords: CL-20; phlegmatizers; sensitivity.

In this work the grain of the ε-CL-20, obtained by precipitation in the different systems of crystallization, were subjected to phlegmatization. Teflon emulsion, synthetic polymer called Viton A, and lacquer on the basis of acetyl butyrate of cellulose was used to the phlegmatization. For all of the obtained samples CL-20 a significant reduction in sensitivity to friction was achieved. The best results were obtained using a Teflon emulsion as a phlegmatizer. However, using phlegmatizers did not cause a significant reduction in sensitivity to impact. Decrease in sensitivity was not significant or remained at the same level. Keywords: CL-20, binders, sensitivity

A novel portable device for fast analysis of energetic materials in the environment

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Keywords: portable device μLC; chemiluminescence; nitramines; nitroesters.

Construction of portable device for fast analysis of energetic materials is described in this paper. The developed analytical system consists of two main parts: a miniaturized microcolumn liquid chromatograph of unique construction and original chemiluminescence detector. This novel portable device is able to determine selectively most of nitramine- and nitroester-based explosives as well as inorganic nitrates at trace concentrations in water or soil extracts in less than 8 minutes.

Research of influence of nozzle geometry on internal ballistics performances of solid propellant rocket motors using numerical simulations

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Keywords: rocket motors; numerical simulation; central convergent-divergent nozzle; multiple perforated nozzles; performance of rocket motor.

For tactical rocket motors with more nozzles allocated in a certain spatial distance from the nozzle axis, the products of combustion after the exit from internal cavity of propellant charge do not enter immediately into the nozzle. Products of combustion are reflected of the nozzle wall, swirling flow in front of the nozzle emerges, and only then products of combustion enter into convergent-divergent conical nozzles. There is a significant change in velocity vector and pressure redistribution of gas flow in region ahead of the nozzle, which bring about changes in development of pressure in rocket motor and change of internal-ballistics parameters, such as total and specific impulse of rocket motor. A better understanding of complexity of gas flow in these cases is possible using numerical simulation. Research was focused to analysis of flow of doublebase propellant combustion products (without metal particles in rocket motors, and the influence of shape of the channel for passage of gases and region in front of nozzle and nozzle geometry to distribution of pressure and flow of the gasses inside rocket motor. For simulation of real gas flow through channel for passage of gases and nozzle, CFD package Comet was used. Using numerical simulations, energy losses in the chanels for passage of gases and in front of the nozzle were estimated. Correlations of individual influences and losses were included in program SPPMEF (authors model for prediction of internal-ballistics parameters of rocket motors), enabling more realistic prediction of internal-ballistics performance of rocket motors.

Numerical simulation of internal-ballistics parameters of solid propellant rocket motors

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Keywords: rocket motors; burning rate; numerical model; compressible flow; transonic flow; boundary conditions; mass flow rate; burning surface.

During the initial phase of design of a solid propellant rocket motors it is necessary to identify and quantitatively estimate deviation of internal-ballistics parameters of observed rocket motors types from ideal conditions. In an initial stage of the design of real rocket motors there are differences between the rocket motor theoretical performances and actual performances based on testing of standard ballistic motors. Therefore modern numerical methods were used as a potential tool for the analysis of characteristics of combustion and gas flow in solid propellant rocket motors with specific design. Numerical simulations provide analysis of certain physical processes in rocket motors, optimizing and reducing the cost of development of new rocket systems (minimizing number of models and tests). Mathematical and numerical 3D model, based on equations of mass, momentum and energy conservation, describing transport processes in rocket motors, is used. Numerical simulation in CFD package Comet (finite volume method) was conducted for real gas flow through the passage channel (for proppelant charge gasses), and in the front and along the nozzle. The results of numerical simulations were verified with theoretical solution for the case of quasi-steady combustion process, with available experimental data of other authors and with our own experimental studies.

A comparison of sensitivity and performance characteristics of melt-pour explosives with TNT- and DNAN-binder

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Keywords: explosive properties; DNAN; TNT composites.

Some sensitivity and performance characteristics for pure 2,4-dinitroanisole (DNAN) and 2,4,6-trinitrotoluene (TNT) as well as for melt-pour composites containing 40 % of DNAN or TNT, 20 % of RDX and 40% NTO were determined (under the same conditions) and compared.

Interaction between tnt and melatonin- dft treatment

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Keywords: melatonin; TNT; DFT calculations.

Abstract: The interaction between TNT and a biologically important molecule, melatonin, has been investigated at the level of density functional theory. The calculations have showed that these molecules in vacuum conditions orient themselves almost parallel, face to face with each other. Various energies, physico-chemical and quantum chemical properties of the system are computed. The calculated electrostatic charges, UV and NMR spectra show the presence of strong interaction between TNT and melatonin. However nature of this interaction (whether an intimate pair or donor acceptor type π-complex formation) is not clear presently.

Numerical analysis of small caliber charge

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Keywords: EFP; explosively formed projectile; shaped charge; computer simulation; Autodyn 2D/3D.

This paper presents a series of optimization studies for the selected charge type of the explosively formed projectile (EFP). The basic version of EFP 45 (caliber charge 45 mm diameter) includes spherical metal liner of copper with a thickness of 2 mm and 80 g of explosive. 2D model of selected charge was constructed by using ANSYS Autodyn 2D – Academic Research Program. All the elements needed to create a model were collected in the program's library: cover charge - POLYETHYL, explosive - PETN 1.77, metal liner - CU-OFHC. After checking the correct functioning of this model it was used to perform further simulations EFP 45 charge for the different variants (additional strengthening of the cylindrical casing charge, the type of the housing material, shape or thickness of metal liner and its density).

The study of the stages of nitration derivatives of 2,6,8,12-tetraacetyl-2,4,6,8,10,12-hexaazaisowurtzitane

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Keywords: product composition; rate of nitration; derivatives of 2,6,8,12-tetraacetyl-2,4,6,8,10,12-hexaazaisowurtzitane.

An HPLC and HPLC-MS study of the product composition and rate of nitration 2,6,8,12-tetraacetyl-2,4,6,8,10,12-hexaazaisowurtzitane, 2,4,6,8,12-pentaaacetyl-2,4,6,8,10,12-hexaazaisowurtzitane, 2,6,8,10,12-hexaacetyl-2,4,6,8,10,12-hexaazaisowurtzitane and 4,10-diformyl-2,6,8,12-tetraacetyl-2,4,6,8,10,12-hexaazaisowurtzitan sulfuric - nitric acid mixtures.

Influence of energetic characteristics of double-base propellants on internal-ballistics parameters

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Keywords: impulse; solid propellant; rocket; internal ballistics.

Solid propellant rocket motors for shoulder launched infantry weapon systems are characterized by short working time, high combustion pressure and large range of designer solutions for rocket motor structure and geometry of propellant charge. Internal-ballistics parameters of impulse rocket motors depend on many factors: design of rocket motor structure, shape of propellant charge, type of connection between propellant charge and rocket motor body, type and position of ignition system, type of motor rotation and nozzle(s) design. Because of enormly high mass flux of combustion products inside rocket motor erosive combustion takes place. Process of ignition signifficantly influences transition combustion process because periods of ignition activation and ignition combustion itself are very similar to period of stable combustion. Considering the fact that these rocket systems should be operative in a broad range of ambiental temperatures (from -40řC to +60řC), types of rocket propellant and ignition system play important role. Type od solid rocket propellant, double-base or composite, or applied technology for manufactoring of propellant charges signifficantly influence internal-ballistics parameters of impulse rocket motors. Double-base propellants are applied in most impulse rocket motors because of their low price, simple manufactoring procedure and low temperature of combustion products. In published literature there are no available models which describes in detail process of design of solid propellant rocket motors and there is very limited number of public refferences with information regarding types of rocket propellants (double-base or composite) used in these rocket systems. Experimental research were conducted in order to investigate influence of ambiental temperature, small changes in energetic characteristics of double-based propellants, and small changes of propellant mass and age of propellant on internal-ballistics parameters of impulse rocket motors.

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