Abstracts of the 20th Seminar on

New Trends in Research of Energetic Materials

NTREM

Pardubice, April 26–28, 2017

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

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Held at the University of Pardubice

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

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NTREM '17

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Preface

The history of NTREM is closely related to the existence of two energetic materials´ research groups based in Pardubice. The first being the Research Institute of Industrial Chemistry practically the research branch of Explosia Co. focusing on industrial and military applications and the second Institute of Energetic Materials (IEM) at the University of Pardubice at that time interested mainly in synthesis and safety in mining applications.

The political changes following the velvet revolution in 1989 affected both of these institutions. The opening of the borders to the west brought a chance to cooperate with new institutions however the transformation from centralistic long term planning of socialistic economy to a newly born market oriented one drastically reduced funding of both of the mentioned institutions. Further the old ties to the East were broken and new ones not established. Both of the institutes were left sort of isolated from international collaborators.

Apart from the financial issues director of the Research Institute of Industrial Chemistry in Explosia Co., Dr. Miroslav Horáček (*sitting in the 1993–2002 period*), correctly identified another important barrier. The employees of the institute were not able to present their results despite being good scientists with many interesting results. They were missing a skill not needed in socialistic Czechoslovakia.

He therefor decided to organize internal seminar at which especially the junior scientists would learn how to present their results in front of the scientific audience. In 1998 students of the IEM were for the first time invited to broaden the list of speakers. This proved fruitfully and IEM was asked to organize the next seminar. Since IEM had newly established collaboration with Military Technical University and Institute of Organic Industry both in Warsaw it seemed logical to invite Polish colleagues. This became known as a second seminar *New Trends in Research of Energetic Materials* shortly NTREM and was attended by 22 Polish, 22 Czech and two Slovak participants out of which 31 presented their work. The similarity of the languages enabled participants to present in their mother tongue.

The third meeting in 2000 was attended by students and experts from the Czech Republic, Egypt, Poland, Croatia, Slovakia and USA. The number of languages proved to be difficult to manage and it was decided to hold the next meeting in English despite the fact that most of the attendees did not poses the skills to comfortably present in this language. It was recognized that the quality of the research is not proportional to the language skills and NTREM should help researchers to get comfortable presenting in English.

It was further decided to emphasize the original idea of enabling students and junior researchers to learn, practice and professionally grow. However to enable participation of students and junior researchers a funding scheme different from the traditional one had to be established. The NTREM has therefore always been open to all free of charge and completely relying on support from sponsors and well established senior participants.

The first NTREM as we know it today was born out of these ideas in 2001.

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
16	2013	25	113	182
17	2014	27	124	203
18	2015	24	98	162
19	2016	28	127	217
20	2017	26	139	~200

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

We should mention here the help obtained from certain individuals—our colleagues from abroad—who have contributed to the creation of the international character of these seminars. From the very first meetings, among the personalities present were professors from the Military University of Technology and also colleagues from the Institute of Industrial Organic Chemistry, both from Warsaw.

Starting with the 4th NTREM seminar, the organisation and management activities related to the seminars have been very actively assisted by Prof. Adam Cumming, nowadays from University of Edinburg in Scotland, and by the late Dr. Fred Volk (*who was a great supporter of young scientists' activities*) from ICT Pfinztal, Germany. Starting with the 5th seminar, Dr. R. H. Woodward Waesche, former editor-in-chief of the Journal of Propulsion and Power, has become another supporter and adviser. The active participation of Prof. Thomas Klaöetke (LMU Munich) and his many students very positively influenced these meetings and showed that scientific results can be presented in an attractive way. In the process of these Seminars development new colleagues appeared in Scientific Committee, from them is possible to mention Prof Tatiyana Pivina from Russian Academy of Sciences, Dr. Muhamed Sućeska from Brodarski Institut in Zagreb, Prof. Michel Lefebvre from Royal Military Academy in Brussels, Dr. Ruth Doherty from University of Maryland, Assoc. Prof. Aleksander Astachov from Reshetnev Siberian State Aerospace University, Prof. Stanislav Cudziło from Military University of Technology in Warsaw, Manfred A. Bohn from ICT Pfinztal and of many other.

The main burden of preparation and organisation of Seminar has traditionally been falling upon Institute of Energetic Materials: Till 2005 a major part of this activity lied on Dr. Jiří Vágenknecht, who left IEM in the same year. In the last ten years thanking must be due above all to chairman of the organizing committee, Dr. Jiří Pachmáň, to members of this committee, especially to Dr. Marcela Jungová, Dr. Iva Ulbrichová and Dr. Jakub Šelešovský and to other members of the IEM staff for their participation on the smooth preparation and running of these meetings. Due to their efforts and also thanks to the level of presented papers by participants of Seminars, inclusive the evaluative and advising activity of Scientific Committee, the involvement in the Seminars NTREM is as follows.

Traditionally, the seminars were sponsored by number of institutions and individuals enabling attendance of wide range of participants, including students and young researchers not yet well financially covered by research grants. For this support we would like to thank all of our sponsors that have decided to support us again this year.

- Office of Naval Research Global, Science & Technology, London
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- Institute of Shock Physics, Imperial College London, UK
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- Faculty of Chemical Technology, Pardubice, Czech Republic

The efficient help in ensuring smooth and successful course of the meeting obtained from all these institutions and also supporters from the Seminar participants is gratefully acknowledged. We greatly appreciate that thanks to this support all the specifics of the seminar can be preserved.

Pardubice, March 22nd, 2017

Zeman

Svatopluk Zeman

Invited Lectures

Energetic materials – past, present and future

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Keywords: future trends; energetics technology.

NTREM is now twenty years old and it is a good time to review the past, see what has been achieved and consider what might happen in the future. This paper will look back with the intention of looking forward and discuss the development of the science and technology. The position twenty years ago may not look so different from the present in some ways; there was and is an emphasis on Insensitive Munitions; an interest in Life Management and also in looking at new materials for possible application. However, these developments will be looked at critically, will be reviewed considering what has not been taken further and what is still developing. For example, in IM there is a far greater understanding of the nature of the problems and greater ability to manage it. There is less reliance on simple' box ticking' and more on the physical understanding of the processes. However, it is not yet possible to model or predict events with sufficiently reproducible accuracy for actual use. It is possible to see trends and fashionable subjects in the last twenty years – where good work in one area has led to others following the line, often with less convincing results. This continues and the challenge is to gain useful information from such areas and develop possible applications in different, productive ways. The community has enlarged significantly; NTREM was a small meeting initially but part of its success has been in opening doors to newer participants and it has done this from the beginning. The changes in the community will be discussed with suggestions on how it might develop further. Finally I will draw some conclusions with a reminder that NTREM has played a major part in the technology.

A focus on fundamentals: elastic response in explosives

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Keywords: elasticity; equations of state.

The current state of research and development in explosive materials is highly dynamic, with many exciting advances occurring in experimental techniques, theoretical understanding, and predictive models. Significant advances have been made in a few decades. In times of such rapid advances, it is important to emphasize fundamentals. Through the example of elastic-plastic response, this paper traces the research history from shock wave profiles in single crystal explosives, through fundamental quasistatic property measurements, to the current state of the art. The importance of basic properties, and fundamentals of the research approach itself, will be emphasized. Large errors in experimental determinations of elastic tensors for these materials had been a serious issue for many years. The collected results and their implications demonstrate the need to keep a focus on the basic properties, and rigorous, careful application of experimental technique and error evaluation.

Nanoparticles for high energy materials.20 years - where we were and where we are going

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Keywords: metal nanoparticles; high energy materials; organic coating.

In the paper review of use of metal nanoparticles as fuel for high energy materials was done. A lot of research group in the World had attempt to replace regular fuel (as a rule microAl) on metal nanoparticles to increase effectiveness of HEMs. It was found the changes for burning rate (the increase), and for index n in burning rate law (conflicting results). Also it is possible to expect the decrease of two-phase losses in the nozzle. In any case all research was done for laboratory scale. In the point of view of authors it is very important to provide a stable characteristics of metal nanoparticles by special chemical treatment for deagglomeration,chemical stability and compatibility. The great attention paid to this problem in the paper moreover that authors possess own production of metal nanoparticles with stable characteristics and with capacity more than 2 tons per year. Data on metal nanoparticles (including bimetal nanoparticles) thermoanalysis are presented. Also effectiveness of the use of metal nanoparticles in model hugh energy materials including data on ignition time and burning rate are analyzed.

Nanoenergetic materials: the perspectives of application in combustion and propulsion

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Keywords: nanomaterials; energetics; propulsion; combustion.

It is known fact that the energy densities of traditional energetic materials are limited by the enthalpies of product species formed, resulting in relatively low volumetric and gravimetric energy densities. Nanoenergetic materials became available last 3 decades and they offer the promise of much higher energy densities and faster rate of energy release. The main idea in energetics is to enhance the surface area and intimacy between reactive components in order to increase the reaction rate and decrease the ignition delay. The energy density in nanoenergetic devices can reach 50 MJ/ kg which is higher by the order of magnitude of that value for combustion of classical propellants. Extremely fast burning rates exceeding 3 km/s can be realized in combustion of porous silicon nanoenergetic composites. In recent years new nanomaterials have been intentionally fabricated or discovered, novel nano-tools have been developed and old ones industrially implemented, and novel properties of the matter at the nano-scale level have been discovered. There still exist a number of unsolved problems in preparation and application of nanoenergetic materials. They relate, in particular, to the questions what is the role of the interface between reacting components and how to predict the reactive behavior in dependency of ignition method, and what is the relationship between nanoparticles size and the composites performance? To get answers, the results of the experimental studies have to be presented in a detailed and concise manner allowing comparison of materials prepared using different manufacturing approaches. Based on critical assessment of available information, the ignition and combustion models will be constructed and reliable predictions of combustion and operational behavior can be made.

Presentations

Prediction of regulation toxicological tests applied to High Energy Molecules

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Keywords: ADMET; computational chemistry.

In collaboration with Airbus Safran Launchers Company (ASL), a research program was set up to have, in the future, optimized tools to predict the toxicity of High-Energy Materials (HEM). The European Union has adopted a legislation about chemicals named REACh (Registration, Evaluation, Authorization and Restriction of Chemicals) to ensure a high level of protection of human health and environment. REACh describes the internationally guidelines of the different toxicological mutagenicity tests like the Ames test. Several in silico methods can be used to predict the toxicity of molecules such as (Quantitative) Structure Activity Relationship ((Q)SAR). The search of structural similarity among molecules is one of the most conventionally used tools in the in silico predictions. The database used in this study compiled available mutagenicity data for the Ames test for a lot of diversified molecules. An explicit list of explosives, from which we know the experimental results of the Ames test in the literature, has been chosen to consolidate the predictive system and validate the predictions. The goal of this study is to use a smarter algorithm to investigate the use of similarity indices and to perform thereafter the QSAR with a software like MOE (Molecular Operating Environment) in order to obtain an efficient prediction tool for different kind of HEMs. All these compounds were evaluated for evidence of potential mutagenicity. This prediction tool will be compared with softwares often used in the scientific community like ACD, PASS or Lazard. This phase allows assessing the prediction's quality. The subject of this paper is to show that our similarity tool can be encoded and applied itself to a wide range of different similarity indices for the prediction of activity of chemical compounds.

Evaluation of concentration, type and particle size of fillers on the dynamic mechanical behaviour of elastomeric HTPB binder

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Keywords: filler effects on loss factor; DMA loss factor modelling; HTPB; filler; AP; Al; RDX.

In a series of investigations, it was found that the second peak of the loss factor curve determined by DMA of HTPB bonded composite propellants and high explosives can change significantly in intensity and shape with composition. Composite propellants with AP connected via bonding agents to the binder matrix can show a pronounced second peak whereas HMX and RDX produce a weaker peak and with high content, it is present only as shoulder. The second peak is also sensitive to ageing and to de-wetting. This means interaction between filler and matrix influence the appearance of the peak. Therefore a more detailed investigation was started to elucidate the influences of fillers on the loss factor curve. Polyurethane binders made from polyol HTPB and isocyanate IPDI were filled with 20, 40 and 60 mass-% of ammonium perchlorate (AP), Aluminum (Al) or RDX, using fine and coarse particles. For obtaining the cured elastomer a special turning device manufactured at Fraunhofer ICT was installed inside the curing oven in order to avoid sedimentation of the fillers during curing. The cured composites were characterized by DMA in torsion mode from 100°C to +70°C, and the quality of distribution of fillers was evaluated by X-ray micro-tomography, which showed homogenous distribution of the filler particles in the samples. The part of loss factor tanδ at lower temperatures originates from the glass-rubber transition of the binder parts unrestricted in mobility. A second broader peak at the high temperature side is caused by binder parts restricted in mobility. The temperatures at each maximum are called Tgunr and Tgres, respectively. The results are: AP and RDX cause more changes in intensity of the first main peak in tanδ than Al particles. The maximum temperature Tgunr is nearly not changed by any of the fillers. The changes in tanδ intensity determined from baseline corrected curves and modelled by EMG (exponentially modified Gauss) distributions indicate that Al has a stronger interaction with HTPB binder than AP and RDX particles. The particle sizes of AP and RDX and their shapes effect the viscoelastic properties. Increasing content of AP and RDX increase the storage modulus G' and somewhat also the loss modulus G'', but as a whole tanδ intensity is lowered in the main peak.

GALCIT projects: the birth of US rocketry

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Keywords: castable solid propellant; storable liquid propellant; galcit; JATO.

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

Solid propulsion for rockets, guns, and gas-generators enjoys unique properties fa-voring its use in space exploration and military missions still for decades to come. Black powder (or something very similar) was invented by Chinese alchemists for medical reasons around 220 BC. Nitrocellulose (NC)-based homogeneous propel-lants were developed in Europe for gun applications during the years 1863-1888. In June 1942 near Pasadena, CA at a site which became later JPL, Parsons succeeded in making the first castable composite solid propellant by combining an organic matrix (asphalt) with a crystalline inorganic oxidizer (KP). Composite propellants eventually replaced black powder and DB propellants in most rocket applications, especially for space exploration missions. The GALCIT Projects carried out at Caltech by the Rocket Research Group can be seen as the most crucial step in the birth of the incredible US rocketry development. This historical survey presents the pioneering projects which started the modern solid rocket propulsion development and also inspired many of the modern liquid rocket propulsion advances. Some hints are also given about the specific contributions and personal destiny of some of the main players of the historical GALCIT Project Number 1.

Influence of various carbon materials on the catalysis of the propellant

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Keywords: double base propellant; combustion; catalyst action mechanism; burning rate; multiwall carbon nanotubes; X-ray electron probe analysis.

The structure and composition of the quenched combustion surface of low-calorie propellant with catalysts (nickel and copper salts) and various carbon materals – carbon black, multiwall nanotubes – have been studied using scanning electron microscopy and X-ray electron-probe microanalysis. It has been established that significant amount of burning rate of the propellant is observed only when there is a carbon frame on the combustion surface is formed and substantial accumulation of the catalyst particles is taken place. Herewith the greater the degree of carbon frame coverage of combustion surface with catalyst, the greater the catalytic effect.

Review of experimental methods to characterise detonation waves in solid explosives

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Keywords: electrical detonators; microdetonics.

The transition to detonation of a solid explosive from a strong shock (SDT) has been the subject of numerous studies. Various methods of producing a suitable shock have been examined, including drop-weight apparatuses, gas guns, laser-driven flyers and electrical detonators. Whilst most of these have been thoroughly analysed there is a lack of conclusive research on the transition to detonation in electrical detonators interferometry techniques such as PDV and VISAR have recently been extensively applied to measure detonation front velocities with great success. The processes used to subsequently infer wave profiles and describe SDT are discussed, as is the dependence of wave profile on confinement, curvature and density. This review is an evaluation of the above methods, their applications and suggestions for the direction of future research in the area.

Where we are, how we got there, and the way ahead from an FOI synthesis perspective

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Keywords: synthesis; review.

This paper describes the trends in the research on synthesis of energetic materials over the decades on a popular scientific note. The trends are illustrated with examples from FOI (the Swedish Defence Research Agency), such as FOX-7 and FOX-12. These two are examples of the trend towards less sensitive explosives, whereas CL-20 is an example of the trend towards higher performance. Other important factors influencing the synthesis of energetic materials at FOI are the focus of the Swedish Armed Forces (SAF), the unfortunate event of terrorist deeds, and environmental and strategic legislation. The most important influence of the work at FOI is the needs of our main customer, which is the Swedish Armed Forces. This paper also contains a summary of the present state of the field and an outlook towards the future.

Synthesis and cocrystallization of bi-1,2,5-oxadiazole nitro derivatives

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Keywords: 1,2,5-oxadiazole 2-oxides; nitrobifuroxan; dinitrofurazanylfuroxan; isomerization; cocrystallization.

A regioselective method for the synthesis of previously unknown bi-1,2,5-oxadiazolyl systems with the 3-nitrofuroxanyl fragment, based on cascade of one-pot reactions comprising acylation of dinitromethane sodium salt with furoxanyl(furazanyl)hydroxamic acid chlorides, nitrosation of the acylation product with NaNO2/AcOH/AcONa, and intramolecular cyclization of the nitrosation product to 3-nitrofuroxanyl moiety, has been developed. It was found that 3-nitrofuroxanyl fragments were capable to isomerize into 4-nitroisomer and 3- and 4-nitroisomeric pair with 3-methylfuroxanyl substituent was inclined to the cocrystals formation with ratio of 3-nitro-:4-nitroisomer = 4:1 and 3:2 depending on the amount of components used for the cocrystallization.

Synthesis and characterization of N,N′-methylene bridged bis(nitropyrazoles)

Dennis Fischer, Jennifer L. Gottfried, Konstantin Karaghiosoff,
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Keywords: energetic materials; nitropyrazole; crystal structure; LASEM.

The preparation and comprehensive characterization of new energetic materials containing N,N′-methylene bridged bis(nitropyrazoles) moiety are reported. The reaction of sodium 4-amino-3,5-dinitropyrazolate (5) with dimethyliodide affords bis(4-amino-3,5-dinitropyrazolyl)methane (6) which can be classified as a thermally stable explosive (T_{dec} = 310 °C). A subsequent oxidation of amino groups using a mixture of sulfuric acid and hydrogen peroxide yields bis(3,4,5-trinitropyrazolyl)methane (7) – a secondary explosive with high nitrogen content (N = 33.50%), good oxygen balance ($\Omega = -11.48\%$; $\Omega_{RDX} = -21.6\%$; $\Omega_{CL-20} = -11.0\%$) and exceptionally high theoretical detonation performance (V_{C-J} = 9304 m•s^{-1}, p_{C-J} = 39.1 GPa; EXPLO5 V6.01). The remarkably high value of calculated detonation velocity was corroborated using the Laser-induced Air Shock from Energetic Materials (LASEM) technique (V_{LASEM} = 9910 ± 310 m•s^{-1}). The reaction of 6 with generated in situ nitrite acid yields the primary explosive bis(4-diazonium-3-nitro-1H-pyrazol-5-olate)methane (8) which shows superior properties than currently used DDNP. Synthesized explosives were characterized by multinuclear NMR spectroscopy, vibrational (IR and Raman) spectroscopy, mass spectrometry and elemental analysis. Low temperature single-crystal X-ray diffraction studies were also performed. The thermal stabilities were measured using differential scanning calorimetry (DSC). The sensitivities to friction and impact were explored. The sensitivity towards electrostatic discharge (ESD) was determined on a small-scale ESD device. The gas phase absolute molar enthalpies at 298.15 K and 1 atm were computed applying the CBS-4M method using the GAUSSIAN 09 program package. Gas phase standard molar enthalpies of formation ($\Delta H_f{}^{\circ}{}_{(g)}$) at 298 K were computed using the atomization energy method. Standard molar enthalpies of formation ($\Delta H_f{}^{\circ}{}_{(s)}$) were calculated using $\Delta H_f{}^{\circ}{}_{(g)}$ and the standard molar enthalpies of sublimation by applying Trouton's rule. By using the $\Delta H_f{}^{\circ}{}_{(s)}$ and the densities, detonation parameters for presented compounds were calculated using EXPLO5 V6.01 thermochemical computer code. The usefulness of reported explosives is represented by their properties (temperature of decomposition, detonation parameters) and facile synthesis route.

Effect of adding 5-aminotetrazole to anthraquinone-free new green colored pyrotechnical smoke formulations

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Keywords: green smoke; anthraquinone-free.

Colored pyrotechnical smoke formulations are predominantly used in the military sector for signaling purposes. Next to an assumed relatively low efficiency in terms of dispersion of the dye, the burning of such formulations results in the contamination of the environment with potential dangerous or toxic materials. Since the dye is the main ingredient in such formulations, initial attempts have been made to replace certain highly toxic anthraquinone dyes, e.g. benzanthrone and vat yellow 4 with more environmentally benign dyes like solvent yellow 33 (SY33), a common drug and cosmetic colorant component. In some cases, e.g. the U.S. M18 green smoke formulation still relies on a mixture of two dyes, SY33 and solvent green 3 (SG3). The available toxicity database of SG3 does not allow a well-grounded hazard evaluation. To tackle the problem of low efficiency, we designed several new green smoke formulations applying 5-aminotetrazole (5-AT) as an additional gas generator. Maintaining the environmental risks in an acceptable range, we applied a 1:1 mixture of copper (II) phthalocyanine (CuPc) and SY33 to produce green smoke. This paper reports the effect of 5-AT on the new green smoke formulations. The percentage of dye in the aerosol was determined by ICP-AES and HPLC-DAD. All formulations were investigated regarding their combustion behaviour as well as their energetic and thermal properties.

Physicochemical properties and exploding action of quite a number of new promising explosives. 1. High explosives

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Keywords: high explosives; physicochemical properties; exploding action.

The great number of different high energy compounds have been synthesized and studied at the Energetic Materials Team of Ludwig-Maximilian University. About forty more interesting and promising such energetic compounds were chosen for more extensive investigation and were conventionally divided into three functional groups. About twenty secondary or high explosives are presented in this first part of investigation. About ten primary or initiating explosives and the same number of energetic plasticizers or plasticizing explosives are presented in the second and third parts. So in this part about twenty more powerful and stable secondary explosives obtained lately are considered. They are 5,5'-bis(2,4,6-trinitrophenyl)-2,2'-bi(1,3,4-oxadiazole) (TKX-55), bistetrazolylamine (H2BTA), diaminouronium 5-nitriminotetrazolate (DAU-NiT), 1-amino-3-nitro-guanidine (ANQ), 1,7-diamino-1,7-dinitrimino-2,4,6-trinitro-2,4,6-triazaheptane (APX), dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate (TKX-50), bis 3,3'-dinitro-5,5'-bis-1,2,4-triazole-1,1'-diolate (MAD-X1), bis(hydrazinium) 4,4'-dinitramino-3,3'-bifurazane ((Hy)2DNABF), bis(3,4,5-trinitropyrazolyl)methane (BTNPM), bis(3,5-dinitro-4-aminopyrazolyl)methane (BDNAPM) and other similar explosives. All these substances are characterized by a number of properties derived from the results of low-temperature X-ray diffraction, infrared and Raman spectroscopy, nuclear magnetic resonance spectroscopy, elemental analysis and differential scanning calorimetry as well by the values of their sensitivity to shock, friction and electric discharges. Molecular properties of considered explosives were determined for isolated molecules and molecular units using quantum chemistry methods implemented in the Gaussian 09 computer program. The B3LYP hybrid functional and the 6-31+G(d) basis set of electron functions were used in most of performed calculations. All the geometric and energetic characteristics of these objects were calculated and the main primary mechanisms of their decomposition were determined. Their infrared and Raman spectra were calculated too. The heats of formation of the explosives were calculated using the CBS-4M method of complete basis set. All parameters of detonation waves and the equations of state for detonation products in the form of Jones-Wilkins-Lee were determined using the EXPLO5 V.6.02 program. Such calculations were performed for different initial densities of explosives and in several cases for various concentrations of binding additives. The calculations of exploding action of examined explosives under different loading conditions were conducted using the ANSYS Autodyn program. Copper barriers were used for a common comparative analysis, and in the several cases, the barriers of various materials in a wide range of changing their dynamical strength were considered too. A complete comparative analysis of obtained results was conducted and the comparison was made with similar results obtained for several classic secondary explosives such as RDX, HMX, HNS and CL-20.

A bioinspired approach to enhancing mechanical and thermal conductivity properties of polymer bonded explosives assisted by polydopamine-coated multi-walled carbon nanotubes

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Keywords: bioinspired; PBX; carbon nanotubes.

When faced with complicated thermal physical environment, the low mechanical and thermal conductivity property of polymer bonded explosives (PBX) could cause severe damage of PBX. Then, improving mechanical and thermal conductivity property is of great importance for PBX. In this study, inspired by mussels, a facile and noncovalent modification for multiwalled carbon nanotubes (CNTs) is adopted by the self-polymerization of dopamine. Then, the polydopamine-coated CNTs (CNTs@PDA) were further incorporated into PBX matrix through water suspension method. Next, in-depth characterizations, including FTIR–FT-Raman–SEM–TEM and TGA, confirmed that the CNTs were successfully coated by a dense graphite-like structure PDA without ruining sidewalls, through the oxidation of dopamine at room temperature. Furthermore, compared to neat PBX and PBX/CNTs nanocomposites, the PBX/CNTs@PDA nanocomposites exhibited improved tensile and compression strength, creep resistance, and thermal conductivity. The work presented herein greatly broadens the application scope of the bioinspired dopamine, and will be potential of interest to the communities in polymer bonded explosives.

A comparison of the mechanical and thermal properties of explosive simulants prepared using traditional and resonant acoustic mixing

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Keywords: RAM.

A Comparison of the Mechanical and Thermal properties of Explosive Simulants Prepared Using Traditional and Resonant Acoustic Mixing. J. Homan1,2, D. Tod1, P.J. Gould1, R. Tunnell1 and W.G. Proud2 1QinetiQ, Fort Halstead, Sevenoaks, Ken TN14 7BP 2Institute of Shock Physics, Imperial College London, London, SW7 2AZ, United Kingdom

ABSTRACT Resonant acoustic mixing (RAM) is a technique that is increasingly used in the energetics community to overcome the issues associated with mixing materials of widely varying properties. This technique is a batch process, where the mixer propagates acoustic energy through a baseplate into a sealed, clamped sample vessel. In comparison to the conventional planetary mixing there are no intrusive mechanical parts and the sample is intimately mixed in a short duration of time.

However, there are questions about how the high intensity of the mixing will affect the overall material properties and ageing characteristics. This paper is the first element of a larger research project, investigating the effect of resonant acoustic mixing on energetic materials. Comparison of RAM-produced materials to conventional planetary mixed compositions is made. Samples consist of hydroxyl-terminated polybutadiene (HTPB) and various loadings of melamine, an inert material which can be used as inert, density simulant in many systems. The resulting materials were studied both mechanically and thermally over a wide range of strain rates and applied temperatures. Increased mixing can result in greater dependence on surface properties and reactivity, a major factor in ageing. Such mixing could potentially also reduce or distribute materials more evenly within a sample thus affecting the mechanical response. This study is underpinned by predictive modelling based on the group interaction model pioneered by members of this research team.

Acknowledgements

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Putting the squeeze on energetic co-crystals: high-pressure studies of 2(CL-20):HMX and CL-20:TNT

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Keywords: energetic; co-crystal; high-pressure; CL-20; HMX; neutron diffraction; Resonant Acoustic Mixing; RAM; TNT.

Two energetic co-crystal systems – 2(CL-20):HMX, and CL-20:TNT – have been investigated under pressure using neutron powder diffraction on the PEARL beamline at the ISIS Neutron Source in Harwell, Oxfordshire; and the results compared in this paper.

As reported in last year's conference, 2(CL-20):HMX was prepared with a ResoDyn LabRAM Resonant Acoustic Mixer using a published method. Smooth compression was observed in this system up to 3.5 GPa, and equations of state were determined, with no observed phase transitions in this pressure range. The bulk modulus of this co-crystal was determined to be intermediate to that of its co-formers.

In this year's work, conversely, anisotropic compression was observed in CL-20:TNT, with a potential phase transition occurring at 4.1 GPa. Structures were refined for each pressure point, and used to derive an equation of state up to 3.6 GPa. In this case, however, the bulk modulus for CL-20:TNT was found to be greater than that of its co-formers, implying a material less compressible than its constituents.

Improvement of electrostatic discharge sensitivity of lead styphnate particles using some polymer coating agents

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Keywords: lead styphnate; electrostatic discharge sensitivity; microencapsulation; Viton; solvent/non-solvent.

This work is devoted to reduce electrostatic discharge sensitivity of lead styphnate as one of the main primary explosives by means of microencapsulation technique involving solvent/non-solvent method in which viton and nitrocellulose used as coating agents. Optical microscopy was employed to examine the coating morphology. The change in quality and sensitivity of lead styphnate particles were studied by using friction, impact, electrostatic discharge and flash point test. The results showed that lead styphnate particles could be effectively coated with viton and nitrocellulose through solvent/non-solvent method without any quality loss in initiating characteristic of lead styphnate. Electrostatic discharge sensitivity test results confirmed the better performance of coated samples with viton respect to nitrocellulose due to conductivity property of copolymer viton. Based on the opti-mization procedure, the most desensitized lead styphnate particles were obtained by using 5% (w/w) of viton as coating agent.

Green synthesis of α-Fe2O3 nanoparticles and their applications on improvement of thermal decomposition and burning rate of solid composite propellant

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Keywords: composite solid propellants; ammonium perchlorate (AP); AP/Fe2O3nanocomposites; catalytic activity; burning rate.

In this research, α-Fe2O3 nanoparticles were successfully produced by high energy ball milling method as safe and environmental friendly process from micronized starting materials. Phase and nanostructure characterizations of the as-crushed powders were performed by using XRD and FE-SEM techniques. It was found that an average particle size of about 40 nm was achieved after 50 hours of process. Then the catalytic activity of the syntheses α-Fe2O3 NPs on thermal decomposition of AP particles and composite solid propellants were investigated by DSC and TGA techniques. Also the burning rate characteristics of the AP based CSPs with and without NPs were measured in Crawford bomb at nitrogen atmosphere based on MIL-STD-286C Method 803.1.1. AP/α-Fe2O3 nanocomposites were prepared by using the solvent-nonsolvent procedure as a fast, scalable and low-cost preparation method. On the other hand, traditional solvent-nonsolvent processes have some serious drawbacks such as the bulk usage of hazardous chemicals and solvents that is undesirable for environmental and industrial applications. Therefore, in the present investigation, some double solvent-nonsolvent system including water-toluene, acetone-methyl ethyl ketone, acetone-ethyl acetate, ethanol-ethanol, water-ethanol and water-water system were investigated based on their efficiency on decreasing the HTD/°C, increasing the ΔH/ J.g-1 and environmental issues. Based on the experimental results, although α-Fe2O3 NPs in water-toluene system illustrate the best catalytic effect containing reduced the decomposition temperature and increases the ΔH of decomposition of AP, but system water-water by reducing the HTD to 370.3 °C and increasing the ΔH to 1050.2 J.g-1, was chosen for the production of nanocomposites from the point of view; efficiency and ecofriendly approach. Finally, the burning rate characteristics of the CSPs with AP/α-Fe2O3 were investigated and the results were shown addition of α-Fe2O3 NPs to CSPs at pressures 41 and 55 bar increased the burning rate from 5.2 to 9 and 5.5 to 10.5mms-1, respectively.

Single-crystal x-ray diffraction (SXRD) studies on energetic materials

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Keywords: sxrd; crystal structure; thermal expansion.

Single-crystal x-ray diffraction (SXRD) is a powerful technique in the structure analysis of crystalline materials, including high explosives and other functional materials. With SXRD, we have solved the crystal structures of two novel energetic complexes, [Ni(en)3]AZT·THF (1) (en=ethylenediamine, AZT=5,5'-azotetrazole, THF= tetrahydrofuran), [Ni(AZT)(pn)2]n (2) (pn=propylenediamine) and two explosive cocrystals, HNS/Bipy (Bipy=4,4'-bipyridine) (3) and HNS/Bipyete (Bipyete=trans-1,2-bis(4-pyridyl)ethylene)(4). In complex 1, the AZT2- anions interacts with the Ni(en)2+ cations via H-bonds, while in complex 2 the AZT2- anions coordinate to the Ni2+ ions to form one-dimensional (1D) zigzag chains. 1 and 2 show prominent effect on the thermal decomposition of RDX, HMX and AP, and have potential applications in propellants. HNS/Bipy and HNS/Bipyete have similar crystal structures, which are formed from the alternatively stacking of HNS layers with Bipy layers and Bipyete layers, respectively. Thermal properties and sensitivity of the two cocrystals have been investigated. Moreover, in-situ SXRD was applied to study the thermal expansion properties of several high explosives including HMX, RDX, TATB and LLM-105.The thermal expansion coefficients of the unit cell parameters have been calculated.

Performance characteristics of a new plastic explosive based on cis-1,3,4,6-tetranitrooctahydroimidazo-[4,5-d]imidazole (BCHMX) and 3-nitro-1,2,4-triazol-5-one (NTO)

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Keywords: bicycle-HMX; NTO; sensitivity; performance; detonation characteristics.

Plastic Explosives have several military and civilian applications. However, high performance with low sensitivity is difficult to obtain using an inert polymeric matrix. In this work, a new plastic explosive composition based on mixture of cis-1,3,4,6-tetranitrooctahydroimidazo-[4,5-d]imidazole (BCHMX) and 3-nitro-1,2,4-triazol-5-one (NTO) bonded by poly-dimethyl siloxane binder (BCHMX/NTO-Sil.),(44/44/12 by wt.), was prepared. For comparison, Two types of plastic explosives based on individual explosives, RDX (1,3,5-trinitro-1,3,5-triazinane or BCHMX, bonded by poly-dimethyl siloxane binder were studied in addition to the commercial available LOVA explosive TNTO (TNT 50% and NTO 50% by wt). Impact and friction sensitivities of these compositions as well as the individual explosives were determined. Experimental detonation velocity were performed for these compositions. Detonation characteristics were calculated using EXPLO5 program and compared with the experimental results. The results showed that BCHMX/NTO-Silicone has low sensitivity in the range of TNTO with higher detonation

A biography of potassium complexes as versatile, green energetic materials

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Keywords: potassium complexes; green energetic materials; crystal structure; energetic three-dimensional metal–organic frameworks.

Potassium-based energetic complexes are environmentally friendly compared to their traditional heavy metal counterparts. They also have higher energy densities and better thermal stabilities than the parent organic compounds due to the deprotonation and introduction of the potassium cation. According to the anion ligands, they can be classified as nitrophenol-, furazan-, furoxan-, triazole-, tetrazole-, and their derivative-based potassium complexes. More than 20 potassium complexes have been prepared, with their crystal structures analyzed and properties characterized, demonstrating their superiority to traditional energetic materials. Multi-coordinated potassium cations facilitate the formation of energetic three-dimensional metal–organic frameworks, making them better candidates as energetic materials for both defense and civil applications.

Characterisation of the thermal and explosive properties of mixtures of EGDN and additional energetic ingredients

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Keywords: EGDN; performance; thermal properties.

Currently, a lot of efforts are put to limit the fabrication of TATP (regulation on the purchase of oxygenated water and other relevant ingredients). One may expect that, in the future, alternative types of homemade explosives will be used for illegal purpose. Ethylene glycol dinitrate (EGDN) belongs to the category of nitro ester liquid explosives. It can be synthesized from easily available precursors (ethylene glycol under various form and nitric acid) and can be therefore used as improvised explosive. The synthesis and determination of explosives performances of EGDN have been previously investigated by H. Fettaka [1]. In this context, mixtures of EGDN and other typical energetic materials have not specifically been studied. Although such investigation is important: - to clearly identify the nature and the magnitude of the potential threat, - to implement technical adequate responses and - to collect relevant data for appropriate regulation. In this investigation, the explosive properties of different mixtures (EGDN + other energetic ingredients) and their thermal characteristics have been studied and will be reported. Using impact sensitivity tests, brisance tests and Differential Scanning Calorimetry, one can identify the influence of the additional energetic materials on the sensitivity, brisance, thermal ignition and thermal decomposition of the different mixtures.

Co-crystallization of energetic materials

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Keywords: co-crystal.

Co-crystallisation is a technique often used in the pharmaceutical industry to tailor properties of materials such as solubility and drug effectiveness. Although widely used in the pharmaceutical industry the technique receives much less attention in the energetic community. Co-crystallization involves crystallization of the energetic material with one or more molecular components in order to tailor, engineer and enhance the properties and performance of the composition for specific applications. Exploiting the concepts of crystal engineering can allow for control over sensitivity of the material, improve performance and alter damage resistance. Having such control over these materials can allow for an enhanced understanding of the effects structural packing can have on properties such as sensitivity.

Interplay of highly accurate quantum chemical computations and thermal analysis techniques in the study of thermochemistry and decomposition mechanisms of energetic materials

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Keywords: quantum chemical calculations; thermogravimetry; energetic materials; formation enthalpies; kinetics of thermolysis.

Modern highly accurate quantum chemical calculations are very powerful and promising complementary tool to experiment in the field of energetic materials (EM). We show two typical applications of quantum chemistry in combination with experimental thermal analysis techniques for particular problems of thermochemistry and kinetics of EM. First, we proposed the convenient and facile procedure to determine the solid-state formation enthalpies of EM. The latter values are obtained as combinations of quantum chemically calculated gas-phase formation enthalpies and sublimation enthalpies obtained from thermogravimetric (TGA) experiments with the aid of the Langmuir equation. Using this technique, we resolved the existing discrepancies in the formation enthalpy of 1,1-diamino-2,2-dinitroethylene (FOX-7). Second, with the aid of quantum chemical calculations, we studied thermal decomposition of tetranitroacetimidic acid (TNAA). TGA and differential scanning calorimetry (DSC) at atmospheric, vacuum, and elevated pressures were used to obtain kinetics of the whole decomposition process. In turn, computations revealed the important role of tautomeric equilibria, and several closely lying radical (C-NO2 bond scission) and molecular (N2O elimination) channels occurring in various tautomers turned out to be dominating primary decomposition reactions of TNAA. The theoretically predicted activation energies (39 kcal/mol) are in perfect agreement with experimental values.

X-ray computed tomography as a tool for 3D assessment of shock tube systems

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Keywords: explosives; nonel; shock wave; energetic systems; XCT.

Shock tube systems are non-electric explosive fuses employed in blasting and demolition applications to trigger the detonation of explosive charges. Their working principle is based on the explosive reaction of a fine explosive powder on the tubing´s inner surface, generating a shock wave traveling at a velocity of 2,100 m/s along the length of the tube, without destroying it. One of the key aspects of the manufacturing process of these shock tubes is the size and morphology of the explosive powder grains and their distribution on the inner wall of the tube, in order to propagate the shockwave efficiently and reliably. This paper introduces X-ray computed tomography (XCT) as a tool for the 3D non-destructive assessment of shock tube systems. This study presents the wide range of parameters that can be measured from a single XCT scan; performing in a single step the characterisation of the explosive powder (grain size distribution, grain shape, grain location), the dimensional characterisation of the shock tube (both inner and outer diameters), and the defect characterisation (presence and location).

Influence of crystal characteristics on the mechanical sensitivities of 2,6-diamino-3,5-dinitropyrazing-1-oxide

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Keywords: explosives; LLM-105; crystal characteristics; mechanical sensitivity.

The sensitivity characteristics of explosives can be related to their chemical as well as physical characteristics including crystal size, morphology, purity, internal and external defects, which play vital roles in the sensitivity of explosives. 2,6-Diamino-3,5- dinitropyrazine -1-oxide (LLM-105) was synthesized and studied intensively as an insensitive molecular explosive. Six types morphologies of LLM-105 crystals with fork , needle, plate, block and flower-like shape were prepared by precipitation crystallization method with dimethyl sulfoxide (DMSO) as the solvent and water,ethyl acetate ,etc. as anti solvent. The morphologies of LLM-105 crystal were performed by scanning electron microscopy (SEM). The whole PXRD and FT-IR spectrums of 6 kinds of LLM-105 crystals are identical and imply that they are the same crystalline form. The impact sensitivity and friction sensitivity were performed by WL-1 and CAST impact instruments and WM-1 type friction sensitivity instrument and give H50 values and explosion probility(%) respectively.The results show that the H50 values and explosion probility(%) were affected by crystal morphology, crystal integrity, particle intra defects and surface smoothness,but hardly have related with particle size, in which, crystal integrity is the key factor influencing the impact sensitivity. The irregular shape including fork and rod and aggregated particles are more insensitive to impact impulse than regular shape which is contradictory to the general law of conventional nitroamino explosives such as RDX,HMX and CL-20. LLM-105 crystals with good integrity and smooth surface and less intra defects are more insensitive to impact which is consistent with the general law of conventional nitroamino explosives such as RDX,HMX and CL-20. The friction sensitivities of all samples didn't changed and showed that the friction sensitivity is mainly attributed to chemical structure of explosive itselfs.

Research on reduced shock technology of laser-driven separation nut

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Keywords: separation nut; pyrotechnic shock; laser ignition; shock absorber.

This Article presents in detail a method of reduce shock of Laser-driven Separation Nut and various shock performance test results of the corresponding samples.In order to improve the safety and reliability of the laser-driven separation nut and reduce the pyroshock of the near field explosion, Firstly, this article gets the limiting charge by calculating the output power of BNCP, as a theoretical basis of reducing explosive load design. Meantime,optimizing the structure of nut by adding special cushion in its internal area of collision between parts, which can effectively damp high-frequency vibration energy caused by release of pre-load strain. Then this article introduces the shock tests of separation nut after optimizing charge mass and structure. According to the digital method for shock response spectrum proposed by Morwood, this article presents the shock data processing procedures in detail. And a data processing program using the MATLAB for it has been worked out. In this article,we get frequency domain shock of release in the X,Y,Z direction maximum is 539,5g(less than 1000g), Verifying the effectiveness of the method.

Oxidation mechanism of micron-sized aluminum particles in Al-CO2 gradually heating system

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Keywords: aluminum particles; core-shell structure; CO2 system; oxidation mechanism.

Micron-sized aluminum powders with different sizes were heated in carbon dioxide atmosphere through differential scanning calorimetry (DSC) method in this work. All samples were analyzed through XRD and SEM which demonstrate that aluminum powders were oxidized into four distinct stages from room temperature to 1500°C. Stage I, amorphous alumina shell turns to γ-Al2O3 phase from beginning to 620°C. Stage II, accompany with the aluminum core melting, alumina shell becomes thicker and fragile at the temperature around 667°C which is the melting point of aluminum. Stage III, in the temperature range of 690-1150°C, alumina shell was broken partially because of the inside pressure. Liquid aluminum core spurts out through the weak cracks on the surface of particles just like volcano eruption and then oxidized by CO2 while the temperature is increased from 700°C to 900°C. Stage IV, alumina composition eventually changes to stable α-Al2O3. From what was presented above, a mechanism of micron-sized aluminum particle oxidation in CO2 under gradually increasing temperature condition was proposed. This model was named “eruption model”, which are responsible for the behaviors that were observed in the experiments.

Self-organized patterns formation and phenomenon of excitation of the unique set of holograms of the energetic materials reactionary zones

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Keywords: micro-scale combustion; reactionary zones; liquid-viscous layer; self-organized patterns; unique set of holograms; combustion enhancement.

The aim of this research is development of the new concept of application of the unique set of holograms of the energetic materials reactionary zones for manipulating by the resonance spectrum of the micro- and nano-scale structures of the reactionary zones. According to our hypothesis each energetic material has a unique set of holograms of the reactionary zones in available specific frequency bands. Our hypothesis is supported by recent data, obtained in the various model experimental systems. In the energetic materials reactionary zones can be observed a unique set of holograms: image, acoustic, electromagnetic and thermal. The analysis of available experimental data show that micro- and nano-scale structures forms both the fractal and self-organized patterns in the reactionary zones and can be considered as a fingerprints of the set of holograms of the reactionary zone. For instance, the condensed particles, existing in the combustion products allows to make physically visible the sound wave patterns. Different frequencies can arrange the micro- and nano-scale structures into the different geometrical patterns. For practical applications in the aerospace propulsion area we suggest new technology of scanning of the multi-component unique resonance spectrum of all molecules in the reactionary zones and programmed transfer of the quantum information into the reactionary zones for excitation of the resonance spectrums of the predetermined set of molecules by means of resonance laser radiation or by use of the system of resonance electro-magnetic and acoustic fields. Such excitation along with re-programming of the resonance spectrum of the micro- and nano-scale structures of the reactionary zones gives the possibility for control by the scale and 3-D localization of the induction and energy-releasing areas and, accordingly, allows control inter-scale interaction in the aerospace propulsion systems.

Subscale motor to investigate the effect of initial temperature on the burning process for solid propellants

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Keywords: burning rate; double base propellant; temperature effect; subscale rocket motor.

The effect of the initial temperature on the burning rate for three compositions of double based propellants (ROP, GRAD 98 and GRAD 06) was characterized. These propellants were fired in a subscale rocket motor and the propellant burning rate was measured as a function of pressure and initial temperature. Variations in the duration of different burning zones were observed. The operating pressure ranges were 5 –24 MPa and the temperature ranges were - 60 °C to +60 °C. It was seen that the increase of the initial temperature of the propellant grain increased the ignitability, burning rate, operating pressure and end burning pressure and consequently shortens the burning time.

Nano- and microthermites for the after-mission destruction of LEO satellite structures during their uncontrolled re-entry

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Keywords: thermite; satellite; re-entry; propellant tank.

The incomplete combustion of the space vehicle in the Earth atmosphere during the uncontrolled re-entry after their mission on Low-Earth-Orbit (LEO) requires a risk of the fall of thermally stable parts on the Earth. In particular, equipment such as titanium tanks for liquid propellants or pressurisation gases are liable not to be destroyed by fusion during re-entry. We propose to reduce this risk by stimulation of the thermal degradation process of titanium propellant tank with the extra-energy supplied by combustion of a pyrotechnic composition. The last is thermite mixture, igniting passively at the altitude with the maximal surface temperature. Once ignited thermite composition will react with the energy release sufficient to melt/oxidize titanium cover followed by the burning out of holes in the wall. Thus intensified ablation/oxidation processes will destruct satellite parts, which in turn will lose their streamline shape, and will be easier burned out being aerodynamically heated during further descending in atmosphere. Our theoretical and experimental studies prove that thermite system comprising of cobalt oxide and aluminum satisfies the stated purpose enabling to be passively ignited by aerodynamical warming-up with the subsequent perforation of the titanium wall. Moreover, tailoring of the aluminum particle size from the nano- to micron-sized and its shape (e.g. spherical or flake powder) allows adjusting the ignition time of thermite system. For thermite formulations with nano-sized aluminum the lower ignition temperature and ignition delay time were obtained compared to that with the micron-sized metal. By controlling the burning time it becomes possible to provide the heat impact at the certain moment of re-entry during deorbiting end-of-life LEO satellites and to reduce the risk of its fall on the Earth.

Macro and microcrystalline waxes: advanced thermokinetic study of evaporation and decomposition under pressure variation

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Keywords: solid fuel; paraffin wax; microcrystalline wax; high pressure DSC; isoconversional kinetics; thermokinetic analysis; evaporation enthalpy.

Paraffin waxes representing mixtures of linear and branched hydrocarbons with diverse carbon numbers are used, among other applications, for solid ramjets and hybrid rocket propulsion. Their utilization assumes the elevated pressure, thus the interplay between evaporation and decomposition becomes important. Using thermogravimetry and differential scanning calorimetry at high pressure, the kinetic parameters for wax pyrolysis were obtained. Paraffin and microcrystalline waxes compared in terms of the evaporation enthalpy and kinetic triplet. The variation of the experimental conditions during thermoanalytical studies shown to effectively probe the kinetics thus highlighting the important distinct steps of the overall process.

Exploring the enhanced reactivity of nanosized titanium toward oxidation

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Keywords: titanium; energetic materials; activation energy; oxidation kinetics.

Nanosized metals establishing the enhanced reactivity are beneficial for various energetic applications. Its current use is limited by the high oxide content and the storage issues – both processes defined by the oxidation kinetics. The oxidation of nanosized titanium was investigated for the first time. Temperature range of the process for nano-Ti is substantially lower than that for micron-sized metal. Kinetic analysis of thermogravimetric data reveals the activation energy of 152 ±3 kJ/mol in agreement with literature reported values. Reaction profile follows the logarithmic oxidation law and its empirical representation for non-isothermal data was proposed. In the absence of unique theoretical description of logarithmic law of oxidation, presented results can promote its development since the effect previously observed on massive plates now is shown on nano-sized particles.

Simulation analysis on cutting capability of flexible linear shaped charge under different bending conditions

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Keywords: flexible linear shaped charge; bending forms; radius of curvature; cutting depth.

Flexible linear shaped charge is often used to cut large metal and non-metallic components with complex structures, and it often needs to be bent to match the structural shape of the components to be cut during use. Under the hypothesis of not destroying the structure of flexible linear shaped charge and liner, LS-DYNA software is used in this paper to study the influence of different bending forms and radiuses of curvature on the cutting capability of flexible linear shaped charge. The research results show that the cutting depth is the largest when the flexible linear shaped charge doesn't bend. The cutting depth increases while the radius of curvature getting large. The outward bending form is significantly influenced by the radius of curvature. When the radius of curvature increases to some particular value, the cutting depth will not change with the increase of radius of curvature. This study can provide theoretical guidance for the design and engineering application of flexible linear shaped charge.

Development of an impact test to study the hot spot formation in PBX

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Keywords: impact; PBX.

The safety of explosives is a topic of prime importance. In this domain, low-velocity impacts are one of the main accidental loadings which can lead to ignition. Nowadays, thanks to the increase of computer's power, we can replace much of the impact test by numerical simulations. Nevertheless, predicting the hot-spot formation in response to mechanical stimuli is sitll very challenging due to the range of complex mechanisms involved in mechanical dissipation. In order to improve our understanding of these mechanisms in Polymer Bounded Explosives (PBX), we develop an impact test that allows observations at the grain scale. Indeed strain localization and the associated generation of heat appear at this scale and they are of prime importance in the initiation process.

In this test, a small PBX sample (10x10x3mm) is confined in an assembly. On one side, a pusher communicates the impact of a hydraulic ram to one face of the sample. We can observe the strain field perpendicularly to the direction of the pusher through a glass window. Compared with previous tests we developed the shape and the material of both the pusher and the confinement assembly to meet our expectations. In that way we ensured that the PBX is sheared under a controlled pressure and that the shear band is localized in the middle of the sample. So we can focus our observations on this area of interest and manage to combine high magnifications for grain-scale observations with fast-camera resolution.

First we develop this test with numerical simulations to determine the strain field for various configurations. Then we verify experimentally the strain field by digital image correlation.

Molecular dynamic simulations of the properties of two poly-(phthalazinone ether sulfone ketone) (PPESK) and the interactions with the TNT

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Keywords: PPESK; TNT; interactions; MD simulations.

The glass transition temperature (T_g) and densities of the poly-(phthalazinone ether sulfone ketone) (PPESK A) are estimated by the plot of temperature with density, volume and free volume, the same properties has been estimated to a novel poly-(phthalazinone ether sulfone ketone) (PPESK B) ,which is designed by introducing nitrol and amini energetic groups in. The estimated T_g and density values of PPESK A is quite closely to the experimental values. Three simulated T_g values of PPESK B obtained by three ways are nearly to each other and about 40 K higher than PPESK A, as it might be the -NH_2 groups are introduced in and the hydrogen bonds are increased, which are mainly leading to the enhancement of the Tg. Three cleaved 2,4,6-trinitrotolluen (TNT) super cells (1 0 0), (0 1 0) and (0 0 1) are interacted with the PPESK A and PPESK B by molecular dynamics (MD) respectively. The cohesive energy densities (CED), solubility parameters (δ),binding energy (Ebind) and mechanical properties are obtained separately. It is implied that PPESK (A or B) and TNT with certain miscibility by difference values of solubility parameters. The values of Ebind of PPESK A/TNT and PPESK B/TNT with the same trend. It is showing that six PBXs models with the sequence as follow: (1 0 0)>(0 1 0)>(0 0 1).By analyzing the PBXs mechanical property (tensile modulus E, shear modulus G, bulk modulus K, Poisson ratio ν and Cauchy pressure C_{12} -C_{44}), because of adding PPESK (A or B) the tensile modulus E of the PBX is lower than pure TNT, that means rigid of the PBXs are reduced. For the ratio values of K/G are all positive value and almost large than that of pure TNT, that is to say PBXs are more flexible than the mono-explosive. Comparing the values of mechanical property of PPESK B/TNT and PPESK A/TNT, the former are commonly larger than later, the mechanical property of PPESK B/TNT are more superior to PPESK A/TNT that mainly for adding the function group nitro (-NO_2) and amino (-NH_2) groups.

On the use of heat of explosion for blast action estimate. Individual explosives and their mixtures

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Keywords: explosives; detonation velocity; heat of explosion; performance; metal acceleration.

Methodological issues of measuring the heat of explosion in a detonation calorimeter are discussed. The heat explosion release time is defined. The equations for calculating the heat of explosion, the detonation velocity and pressure, the relative throwing ability of individual explosives and their mixtures as a function of their chemical composition are derived. The obtained heat explosion release time and the statistical analysis of correlations between various detonation parameters of explosives demonstrate that the heat of explosion serves as a suitable and convenient measure to calculate detonation parameters and to describe the performance of high explosives.

Acceleration ability of HMX-based plastic-bonded explosives

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Keywords: acceleration ability; HMX-based PBXs; Gurney energy; conversion efficiency.

This article aims to present a systematic study on the acceleration ability of a series of HMX-based PBXs with the mass content of HMX (C_{HMX}) from 84% to 95% and also intends to give a reasonable model with physical meaning for accurate prediction of acceleration ability of the explosives. For this purpose, the fundamental detonation parameters, such as detonation velocity D_{CJ} and detonation pressure p_{CJ}, of the PBXs have been experimentally measured, the Gurney energy E_G and Gurney velocity, the important indicators for acceleration ability, have been obtained by the cylinder test. From the viewpoint of energy conversion efficiency, a correlation which link E_G to the initial density ρ_0, D_{CJ} , p_{CJ} and A , a coefficient indicating the conversion efficiency of the released internal energy during detonation into the kinetic energy of the accelerated metals and the detonation products, has been deduced from the basic relations of shock waves and the Chapman-Jouguet (C-J) hypothesis. Based on the experimental data, the value of A is acquired. As the cylinder tests only give information of the radial acceleration ability, the axial acceleration plate flyer tests were also carried out to validate the correlation, the results show that the plate velocities predicted by the correlation are in good agreement with the measured values, indicating that this correlation is suitable for the prediction of both radial and axial acceleration ability of the PBXs. These results not only give a deeper insight into acceleration ability of the HMX-based PBXs, but also allow for the efficient design of PBX formulations, by providing a method to predict acceleration ability of a design prior to experimental validation.

A comparative investigation on underwater explosion energy output of CL-20 and HMX-based aluminized explosive

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Keywords: CL-20-based aluminized explosive; HMX-based aluminized explosives; underwater explosion; energy output.

The underwater explosion output characteristic of CL-20 and HMX-based aluminized explosive is investigated through underwater explosion experiment. The formulas are in the same Al/O ratio but different explosive mass fraction. The shockwave overpressures pm and the energy release are analyzed according to the experiment data. The result shows that, with the explosive mass fraction changing from 10%-30%,pm in the same distance grows gradually, and shock wave energy Es increases. The bubble energy Eb and total energy E climbs up and then declines, which are highest at 20%. So the optimal explosive mass fraction of explosive/AP(ammonium perchlorate)/Al formulas is 20% when the Al/O Ratio is 0.71. The energy release of CL-20 formulas is more than HMX formulas. Es is 9.3% higher; Eb is 4.8% higher; and E is 6.1% higher. The result shows CL-20's energy superiority as a new energetic material, so there is a promising application prospect of CL-20 formulas in aluminized explosive used for Underwater weapon.

Preventing irreversible growth of DNAN by controlling its polymorphism

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Keywords: 2,4-dinitroanisole; DNAN; thermal growth; crystal doping; polymorphism.

Up to 15% irreversible growth of DNAN has been previously observed when the ma-terial is temperature cycled from -54 oC to +71 oC, whereby less than 1% is consid-ered acceptable. We have discovered a complex system of polymorphism in DNAN, with one notable transition occurring within the temperature cycling regime at -7 oC. This disorder-order phase transition from DNAN-II to III involves a notable jump in the unit cell volume and has been found to be the major cause of the growth experi-enced with DNAN. Doping the crystal structure of DNAN with molecularly similar materials is able to suppress this II-III transition to outside the temperature cycling regime. Doping with ‘EDX-1’ is able to eliminate the transition to below 150 K. When samples of DNAN doped with EDX-1 are temperature cycled, the II-III transition is no longer encoun-tered and more importantly, irreversible growth is no longer observed. Through these studies we have developed further understanding of DNAN which has the potential to help enable DNAN to be used as a less sensitive replacement for TNT in melt-cast formulations.

Molecular dynamics simulation study of the effects of crystal structures on the sensitivity of explosives

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Keywords: sensitivity; co-crystal; dislaocation defects; MD simulations.

Abstract: Sensitivity mechanism is a crucial but very complicated topic in the field of energetic materials, which depends on the multilevel structures of energetic materials, external stimulus, and environmental conditions. At the crystal level, the crystal stacking mode, defects, crystal shape and size can affect the sensitivity.1–4 In this work, the effects of structure of co-crystal and disloaction defects on the sensitivity of explosives were studied by the molecular dynamics simulation with ReaxFF forcefied. For details, the thermal decomposition of CL-20/HMX co-crystal and pure crystal of CL-20 and HMX were studied. The potential energy evolution, reaction mechanisms, species analysis and cluster evolution were discussed. Our results show that The decay rate of CL-20 in co-crystal becomes slower compared with pure single crystal; on the contray, the decay rate for HMX becomes faster. This result implys that the thermal sensitivity of CL-20/HMX co-crystal is intervenient between pure crystal of CL-20 and HMX. Moreove, the chemical responses of shocked dislocation-contained and perfect RDX crystals were also studied by the MD simulations. In view of the evolution of temperatures, pressures and reactant decay rates of the shocked perfect and dislocated RDX, we confirm that all dislocations enhance the shock sensivitiy of RDX, and the edge dislocations do it evidently, while screw dislocations mildly.

Numerical simulation and experimental study on double-layer shaped charge liner

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Keywords: double-layer shaped charge liner; numerical simulation; jet; X-ray photograph.

Compared with traditional shaped charge liner, the mechanism of energy absorption and conversion of double-layer shaped charge liner (DLSCL) is more reasonable, and chemical energy is used more fully, significantly improving the projectile's penetration capability. In this paper, LS-DYNA software is used to analyze the properties of the DLSCL. The influence of different materials on the jet shape, jet tip velocity of DLSCL is studied. The results show that when the inner liner is Cu and the outer liner is W, the jet tip velocity reaches the maximum. On the basis of the pulse X-ray photograph, the formation process of the DLSCL is researched. The simulation and experimental results are in good agreement that can provide references for studying and designing the DLSCL.

Thermal behaviors of TKX-50: Experiments and simulations

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Keywords: TKX-50; thermal behavior; proton transfer; simulations.

Dihydroxylammonium 5,5’-bistetrazole-1,1’-diolate (TKX-50) is an important representative of energetic ionic salts (EISs) and outperform many common explosives. We report for the first time a solid-solid phase transition of TKX-50 to a new metastable phase (Meta-TKX-50) at 180 oC, by Raman spectroscopy and TGA-DSC measurements, in combination with ab initio calculations. Meta-TKX-50 is formed by the rotation of NH3OH+ with a small volume expanding of 3 % and a crystal symmetry reduction from P21/C to P-1. In addition, the phase transition of TKX-50→Meta-TKX-50 features a second order one with a slight change of 0.3 J·K-1·mol-1 of. This is the main reason for that it was overlooked in the past measurements. Besides, the transition facilitates the H-transfer from NH3OH+ to C2O2N82- and the N-O bond dissociation of NH3OH+ to produce small stable molecules of NH3 and H2O. Thus, the phase transition is expected to promote the decomposition of TKX-50 deteriorate its thermal stability. Also, we confirms the occurrence of a reversible proton transfer (RPT) during heating and cooling of TKX-50, by means of temperature-variable single-crystal X-ray diffraction and ab initio molecular dynamics simulations. The RPT occurs between the cations and anions of TKX-50, accompanied by energy transfer. More importantly, the RPT is a new sensitivity mechanism for energetic materials against external mechanical stimuli. Chemically, the RPT buffers against external stimuli by reversible chemical reactions, i.e., external mechanical energy is dispersed from mechanical energy to heat, chemical energy (storing and releasing), and then heat release to environment after unloading. Such RPT mechanism elucidates the low impact sensitivity of TKX-50, which is difficult to be explained by existing theories, such as molecular stability and molecular stacking mode in crystals. Accordingly, a novel strategy of ready reversible reactions is proposed for developing insensitive energetic materials and desensitizers. This work provides an exception of prior reactions favoring high safety of energetic materials, relative to those that mostly result in irreversible and hazardous consequences. Thus, this study extends the fields of both proton transfer and energetic materials.

Intermolecular interactions in a hydrogen-free molecular crystal

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Keywords: hydrogen-free molecular crystals; benzotrifuroxan; intermolecular interaction.

Hydrogen-free molecular crystals are generally energetic materials with good detonation performance and extremely high explosion temperature. However, it is still not understood that, without hydrogen bonding and strong charge-induced dipole interactions, how do the nonpolar molecules interact to stabilize the associations into a preferred crystalline structure with a specific performance. Using a widely used explosive benzotrifuroxan, we make insight of the origin of intermolecular charge transfer and the driving force of a pre-ferred T-shaped crystalline structure. The major difference of the π-stacking confor-mations between the hydrogen-free and hydrogen-involved systems is also proposed. The original nonpolar molecules become polar in crystals due to anisotropic molecular inter-actions which break the original symmetry of electronic distribution. The consequent di-pole-dipole interaction is a non-negligible factor of intermolecular attraction. We have al-so demonstrated the strengthening of σ bonds and the weakening of π bonds of the ben-zene ring in the π-stacked system, as well as the electrostatic repulsion at all the intermo-lecular local contacts of a CNO molecular crystal. All these atomistic characters are the reasons of the high level of detonation performance but low level of safety of this kind of energetic materials.

Influence of purification of energetic binders by vacuum rotary evaporation in different conditionse

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Keywords: energetic binders; glycidyl azide polymer; vacuum rotary evaporation; vacuum stability.

Some low molecular weight solvents residual during the synthesis process of glycidyl azide polymer(GAP)which is a potential energetic binder for rocket propellants or cast-cure PBXs may affect the performance of energetic compound. In order to satisfy the requirements of stability, vacuum rotary evaporation with different conditions were used to purify the energetic binder and plasticizers. By comparing the key properties of the energetic binders before and after purification, we found that, binders after purification by specific conditions can meet the requirements of propellants or explosives. The vacuum stability of energetic binders was promoted greatly and the hydroxyl value was seldom influenced under the condition of -0.085MPa, 90°C and distillation for 3 hours.

Posters

New smokeless double-base propellants based on oxalate, nitrocarbamate and formate

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Keywords: smokeless DBP; BTNEO; TNENC; TNEF.

The preparation and characterization of three different formulations of new high-performance smokeless double-base propellants based on the trinitroethyl unit is reported. The new ingredients are: bis(2,2,2-trinitroethyl)oxalate [BTNEO], 2,2,2-trinitroethyl-nitrocarbamate [TNENC] and 2,2,2-trinitroethyl formate [TNEF]. The investigated formulations showed high performance parameters and good thermal stability with homogenous smokeless burning and high density. The higher decomposition temperatures of the three different compositions 186, 153 and 192°C respectively give them higher thermal stability compared to the decomposition temperature of NG (40°C) in the ordinary DBP formulation. The composition which was based on carbamate (NC/TNENC) showed the highest burning rate, followed by the composition which was based on formate (NC/TNEF) while the lowest burning rate was observed using the composition which based on oxalate (NC/TNEO). On the other hand, the highest burning temperature was found for the composition NC/TNEF, followed by NC/TNENC. Also, the high densities of the three new ingredients (BTNEO, TNENC and TNEF) which are (1.84, 1.73 and 1.81 g.cm-3 at 298 K, respectively) give the propellants high loading densities in the rocket motor in comparison with the density of NC (1.59 g.cm-3 at 298 K) in the ordinary DBP formulation.

Flexible linear shaped charges for underwater cutting

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Keywords: plastic explosive; Munroe effect; water pressure.

The flexible linear shaped charge system fabrication and use frame one of the main directions of the Romanian Defense Industry development. The operations of rapid cutting/perforation of metallic structures found in water are mandatory during crisis situations, such as fast release of the navigation channels/fairways of sunk boats wrecks, operations on petroleum pipes or underwater drilling platforms, etc. From both military and civilian point of view, the flexible linear shaped charges provide a great advantage to the EOD staff acting under the water, when the outcome imposes a rapid penetration in sunk containers, the rapid disposal of obstacles, or in combat situations or intervention for countering terrorist actions.

The kinetics of hydrolysis of 4-nitrosemicarbazide and its salts

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Keywords: nitrosemicarbazide; S-methyl-N-nitroisothiourea; 3,5-dinitrimino-1,2,4-triazole; kinetics of hydrolysis; activation parameters.

Reaction of S-methyl-N-nitroisothiourea with salts of 4-nitrosemicarbazide proceeds with formation salts of 3,5-dinitrimino-1,2,4-triazole. In this reaction, the salts of 4-nitrosemicarbazide are a source of hydrazine. The rates of hydrolysis of 4-nitrosemicarbazide and its salts have been measured at interval between 70 and 100 degrees by UV spectroscopy method. The kinetic and activation parameters are determined and reaction mechanism has been proposed.

Reaction of S,S'-dimethyl-N-nitroimidodithiocarbonate with nitroaminoguanidine

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Keywords: S,S'-dimethyl-N-nitroimidodithiocarbonate; nitroaminoguanidine; nitroguanylhydrazone.

Reaction of S,S'-dimethyl-N-nitroimidodithiocarbonate with nitroaminoguanidine has been investigated. Surprisingly found that the nucleophilic substitution reaction proceeds with the substitution of the nitroimine group of S,S'-dimethyl-N-nitroimidodithiocarbonate instead methylthio groups. The reaction product is nitroguanylhydrazone of S,S'-dimethyldithiocarbonate. Structure of the compound is established by X-ray diffraction, NMR spectroscopy, mass spectrometry and elemental analysis, as well as studied by FTIR and UV spectroscopy.

Kinetic study on GAP base copolymer

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Keywords: poly(glycidyl azide); poly(caprolactone); kinetic study; FWO method; activation energy.

Although GAP is a well-known and promising energetic polymer, propellants based on it suffer from poor mechanical and low-temperature properties. To overcome these problems, GAP-based copolymeric binders were prepared and investigated. An energetic triblock copolymer PCL-GAP-PCL was synthesized by ring-opening polymerization of ε-caprolactone by low molecular weight glycidyl azide polymer (GAP) macromolecule as initiator and catalyzed by dibutyltin dilaurate (DBTDL) at 100 °C without the solvent in two steps. Products obtained in high yields (91.12%) were characterized by FTIR, gel permeation chromatography (GPC) and 1H NMR and 13C NMR spectroscopy. Thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) were used to study the thermal decomposition behavior. An advanced isoconversional method has been applied for kinetic analysis. Activation energy calculated by Flynn-Wall-Ozawa (FWO) and Thermal analysis revealed that triblock copolymer has more thermal stability than the homopolymer of GAP. The result of activation energy from Kissinger method for the first and second step were 180.3 and 209.8 kJ.mol-1, respectively. Also, it was found from FWO, the activation energy for the copolymer increased as the degradation proceeded. The glass transition temperature (Tg) for GAP was influenced by the molecular weight of GAP and PCL blocks. Tg of GAP with low molecular weight and copolymer were -60.3 °C and -64.3 °C, respectively as result copolymer showed better thermal properties than the GAP.

The synthesis of novel energetic salts based on N-(1-carboxymethyl-1H-tetrazol-5-yl)-hydrazinium

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Keywords: aminotetrazole; hydrazinium salts; nitroiminotetrazole; energetic compounds; nitrogen salt formation.

One of the overall goals of energetic materials, synthesis of materials with acceptable performance and low sensitivity to physical stimuli. Since the creation of networks of hydrogen bonds, good stability of the triggers may be created and on the other hand azole-based ion high-energy materials (especially aminotetrazole) and other nitrogen-rich compounds that have a strong hydrogen bonds, Significant stability and insensitivity to physical stimulus and also have a good performance. The nitrogen rich compounds are often different from conventional explosives such as TNT, TEX, CL-20 and HMX. Energy of nitrogen rich compounds are obtained from the high positive heat of formation (ΔHf), while the second category of energy from the oxidation of their carbon body and the pressure cage. Studies have shown that the incorporation of hydrazino groups into a tetrazole ring will increase the heat of formation of the molecule and increase the intra and intermolecular hydrogen bonds, which density increases and decreases sensitivity. Also nitroiminotetrazole and their derivatives suitable for high explosives because they combine both the strongly oxidizing and the energetic nitrogen-rich backbone in one molecule. this combination produced a very simple, safe and is inexpensive. Hence, the industry is very important. In this study after the Synthesis salt of N-(1-Carboxymethyl-1H-tetrazol-5-yl)-hydrazinium chloride, the reaction of anion exchange of chlorine with nitrate, 5-aminotetrazolate, (5-Amino-tetrazol-1-yl)-acetate and (5-nitroiminotetrazole-1-yl)-acetate and formation AgCl precipitate, salts to be synthesized and analysis of all products produced using 1H NMR,13C NMR, IR and UV-Vis identified and verified. among the advantages of this study, the use of methods and equipment available and low-risk solvents during the reaction and achieve at least the byproducts of the process took place

Modeling of the nitration of 2-methylpyrimidine-4,6-dione (MPD)

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Keywords: MPD; modeling of the nitration; kinetics.

In this work the conditions and kinetics of nitration of 2-methylpyrimidine- 4,6-dione (MPD), which leads to the formation of 1,1-diamino-2,2-dinitroethene (DADNE, FOX-7), are presented. An analysis of literature data enabled us to propose a simple model of the nitration of MPD. The model was verified on the basis of literature data and our own experimental data. The influence of the rate of nitric acid additioninto a model reactor on temperature and composition of the reaction mixture was investigated. The proposed nitration model could be useful in a study of the MPD nitration process on a large scale.

Detonation velocity of different nitrocellulose based propellants

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Keywords: detonation velocity; propellants; nitrocellulose.

Research on detonation properties of different nitrocellulose based propellants was conducted. Cylindrical charges with propellants containing nitrocellulose and nitroglycerin were considered in this study and experimentally measured detonation velocities are presented. Experiments were done using different measuring methods. Second part of this study was focused on possibilities of reliable detonation velocity prediction. Different calculation methods were used and results were compared with experimental data.

Use of a nitric acid salts in the heterogeneous solid rocket propellants with low HCl content in combustion products

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Keywords: HTPB; nitric acid salts; burning rate; heterogeneous solid rocket propellants.

This paper reports on use a nitric(V) acid salts in heterogeneous solid rocket propellants based on HTPB/AP system with low content of HCl in combustion products. By ICT-Code program were determinate theoretical values of thermochemical and thermodynamical properties like isochoric heat of combustion (Q), specific impulse (Isp) and combustion products in chamber and nozzle of the rocket motor. Authors chosen 5 composition of the heterogeneous solid rocket propellants with 0.3-1% HCl content in combustion products and casted them in laboratory scale. The obtained propellants were combusted in laboratory rocket micromotor for the examination of ballistic properties. By experimental methods were determinate rheological properties and such parameters as: isochoric heat of combustion, sensitivity to mechanical stimuli and decomposition temperature.

Dinitropyrazoles as advanced energetic materials

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Keywords: explosives; pyrazoles; nitrogen-rich; sensitivity; crystal structure.

The syntheses of several 3,4- and 3,5-dinitropyrazoles are described and compared to each other. Several nitrogen-rich salts were synthesized in order to tune performance and sensitivities values. Obtained compounds were characterized using low temperature single crystal X-ray diffraction, vibrational (IR, Raman) spectroscopy, multinuclear NMR spectroscopy, mass spectrometry, elemental analysis and differential scanning calorimetry (DSC). The sensitivities toward external stimuli (impact, friction and electrostatic discharge) were determined according to Bundesamt für Materialforschung (BAM) standard methods. The energetic performances were calculated using the EXPLO5 code and support the high energetic character of the title compounds. Heats of formation were computed by the atomization method based on CBS-4M electronic enthalpies and heat of combustion were determined by bomb calorimeter measurements.

Pyrometers - devices for non-contact measurement and display of energetic materials temperature. Performance improvement

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Keywords: pyrometer; infrared; radiation; temperature; measurement; noncontact.

In the process of creating new and improving existing pyrometers following problems have to be solved. The first one is improving the accuracy of measurement and reduction of timing of radiation absolute temperature. We have solved this problem by using more advanced high-sensitive pyroelectric detector. It provides temperature differential lock to 0.1 K. High limit of measurement has increased up to 3800 K. The new controller allows shorten the time framed up to 0.2 ms. The second solved problem is the generation of acoustic and light alarms in case of deviation of material temperature from the setpoints. Inbuilt interface allows transmit an alarm signal to the system of entire technological process control. The new pyrometer represents a significant step forward in the design of this type devices.

Estimation of sensitivity indicators of solid HE to impact

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Keywords: high explosives; mixed explosives; sensitivity to impact; indicators calculation.

The method of parameters estimation of solid HE and mixes of type HE-HE to impact on drop-weight machine, based on thermodynamic relation of thermal energy and pressure in a deformable charge and the solving of the kinetic equation connecting local HE warming up with time of test charge destruction is offered. The good agreement of calculated and experimental results is observed.

Simulation and optimization of hydrocarbons gas phase partial oxidation in a closed unsteady reactor with adjustable volume

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Keywords: periodical reactor; perfect mixing; adjustable volume; hydrocarbons; partial oxidation; optimization.

It is considered one of the typical technological schemes of gas phase chemical reactor - a closed periodical reactor of ideal mixing with the ability to control changes in the volume of time. This scheme is of interest both for the energy and chemical technology, but much less studied than the traditional scheme stationary flow reactor. In this paper a mathematical model describing abstract periodical reactor with a variable volume and multi-component gas-phase reactions of general type. The model is used to numerically study the oxidation of light hydrocarbons in the framework of the kinetic C1-C2 scheme of elementary reactions. Partial oxidation is investigated for a wide range of process conditions. One consider the aspects of optimization the target chemical, power and dynamic performance

Green-burning pyrotechnic flare formulations based on amorphous boron

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Keywords: pyrotechnics; green light; amorphous boron; burn time.

Traditionally, in pyrotechnics green light with a dominant wavelength around 560 nm and a color purity in the 60 % range is produced by burning mixtures of the green color imparter barium nitrate, magnesium fuel, and a chlorine donor via the formation of metastable barium(I) chloride. However, barium compounds induce muscle cramps and adversely affect the airways and the heart function. Furthermore, commonly used perchlorate oxidizers are associated with malfunctions of the thyroid gland and combinations of such salts with organic moieties as well as organochlorine materials such as polyvinyl chloride often serving as chlorine source combust to highly carcinogenic polychlorinated aromatic compounds. When amorphous boron is burned together with an oxidizer, it forms metastable boron oxide with similar emissive properties. In contrast to barium nitrate, amorphous bo-ron and its combustion by-products can be classified as less toxic and the generation of the species responsible for the emission of green light in amorphous boron-based pyrotechnics does not require the presence of chlorine. Nevertheless, such mixtures burn down too fast due to the especially high flame temperatures generated. With the aim of developing long-burning pyrotechnic formulations using amorphous boron as green color imparter, various oxidizers were tested in combination with tetramethylammonium nitrate. The dominant wavelengths, color purities, and burn times as well as the thermal stabilities and energetic properties of the most promising test formulations were measured. Furthermore, information on ongoing research is given.

Optimization of SPME for determination of nitro compounds using GCMS

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Keywords: SPME; GC-MS.

SPME is extraction technique, which is compatible with gas chromatography. The sensitivity may be good for determination of very low concentration levels. In this paper is this method used for determination of aromatic nitro compounds. Mixtures of aromatic nitro compounds and concentrated nitric acid are potentially useful as home-made bomb. Therefore, it is necessary to find sensitive analytical procedures for the determination of residues after the explosion. Connection gas chromatography with mass detector was used for analysis. It is necessary to optimize conditions SPME (time, temperature, sorption and any amount of NaCl). To optimize the use of statistical techniques DEO. Suitable extraction conditions were found with this method. These conditions were tested on real samples after the explosion.

Mechano-chemical analysis of elastomeric gycidyl azide polymer networks

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Keywords: GAP; Network.

Glycidyl azide polymer (GAP) networks were prepared using hexamethylene di-isocyanate (HMDI) and trimethylol propane (TMP) at different NCO/OH ratios. The number average molecular weight between junction points of the networks (Mc) was calculated using the data obtained from equilibrium swelling experiments in THF at 45°C. It was observed that the Mc, sol fraction and stress-strain behaviors of the networks were profoundly influenced by the cross-link density. Dynamic mechanical analysis (DMA) of the networks was performed between -120°C and 0°C and segmental motions of pendant azido-methyl groups were detected at -107°C.

Molecular properties and primary decomposition mechanisms of several tetrazolatoamminecobalt(III) perchlorates

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Keywords: tetrazolatoamminecobalt(III) perchlorates; molecular properties; primary decomposition mechanisms.

The work is a continuation of a series of studies on the chemical and molecular properties of a number of tetrazolatoammine cobalt (III) perchlorates, which are used as the main components in primary initiating and light-sensitive explosives. Results of a large number of quantum-chemical calculations of isolated molecular units of such substances as 2-(5-cyanotetrazolato-N2) tetraamminecobalt(III) perchlorate (CP), (5-nitrotetrazolato-N2) pentaaminecobalt(III) perchlorate (NCP), cis-bis-(5-nitrotetrazolato-N2) tetraamminecobalt (III) perchlorate (BNCP) and bis-(1-methyl-5-aminotetrazole-N3, N4) tetraamminecobalt(III) perchlorate (TCP) are presented in the paper. The products of their possible primary stages of decomposition are considered too. Molecular properties of exanined explosives were determined with the use of quantum chemistry methods implemented in the Gaussian 09 computer program. The B3LYP hybrid functional and the 6-31+G(d) basis set of electron functions were used in most of performed calculations. A simpler 3-21G basis set was utilized for performing a large number of preliminary and auxiliary calculations. In particular, this basis set was useful for a large number of calculations of various ways of decomposition reactions. The calculations were performed for the molecular units not only in the basic state but also in excited and charged, positively and negatively, states. All geometric and energetic characteristics of considered objects were calculated and the main primary mechanisms of their decomposition were determined. Such characteristics as the total electron energies of molecular units, their zero-point energies, atomization energies, the distributions of electron density, the structures of the highest occupied and lowest unoccupied molecular orbitals and appropriate HOMO-LUMO energy gaps were obtained and presented. The infrared spectra for all molecular units and fragments formed during decomposition were calculated too and were compared with experimental results for crystalline lattices. All possible decomposition mechanisms were considered but tearing off an ammonia molecule from the molecular unit had the lowest levels of activation and dissociation energies and was accepted as the prevailing one. This mechanism among other things was accompanied in most cases by simultaneous molecular rearrangement of the remaining fragment of the molecular unit. The activation and dissociation energies were examined for this and other less possible primary decomposition mechanisms such as tearing off various molecular fragments from the molecular units and rupture of the weakest link in a tetrazole ring. Such decompositions mechanisms can in principle also take place under certain conditions of intensive loading.

Physicochemical properties and exploding action of quite a number of new promising explosives. 2. Primary explosives

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Keywords: primary explosives; physicochemical properties; exploding action.

The great number of different high energy compounds have been synthesized and studied at the Energetic Materials Team of Ludwig-Maximilian University. About forty more interesting and promising such energetic compounds were chosen for more extensive investigation and were conventionally divided into three functional groups. About ten primary or initiating explosives are presented in this second part of investigation. They are 1,5-di(nitramino)tetrazole (DNAT), 6-diazo-3-hydroxy-2,4-dinitrophenol (DHDNP), diazidoglyoxime (DAGL), calcium-5-nitraminotetrazolate (CaNAT), potassium 1,1'-dinitramino-5,5'-bistetrazolate (K2DNABT) and other similar explosives. All these substances are characterized by a number of properties derived from the results of low-temperature X-ray diffraction, infrared and Raman spectroscopy, nuclear magnetic resonance spectroscopy, elemental analysis and differential scanning calorimetry as well by the values of their sensitivity to shock, friction and electric discharges. Molecular properties of considered explosives were determined for isolated molecules and molecular units using quantum chemistry methods implemented in the Gaussian 09 computer program. The B3LYP hybrid functional and the 6-31+G(d) basis set of electron functions were used in most of performed calculations. All the geometric and energetic characteristics of these objects were calculated and the main primary mechanisms of their decomposition were determined. Their infrared and Raman spectra were calculated too. The heats of formation of the explosives were calculated using the CBS-4M method of complete basis set. All parameters of detonation waves and the equations of state for detonation products in the form of Jones-Wilkins-Lee were determined using the EXPLO5 V.6.02 program. Such calculations were performed for different initial densities of explosives. The calculations of exploding action of examined explosives were conducted using the ANSYS Autodyn program. Copper barriers were used for a common comparative analysis, and the barriers of several secondary explosives, RDX first of all, were used for a comparative analysis of their initiating ability. A complete comparative analysis of obtained results was conducted and the comparison was made with similar results obtained for several classic primary explosives such as lead azide, lead styphnate and tetrazene.

Physicochemical properties and exploding action of quite a number of new promising explosives. 3. Plasticizing explosives

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Keywords: plastic explosive; physicochemical properties; exploding action.

The great number of different high energy compounds have been synthesized and studied at the Energetic Materials Team of Ludwig-Maximilian University. About forty more interesting and promising such energetic compounds were chosen for more extensive investigation and were conventionally divided into three functional groups. About ten energetic plasticizers or plasticizing explosives are presented in this third part of investigation. They are 1,3-dinitramino-2-nitroxypropane (NG-N2), N-methyl-N-(2-nitroxyethyl)nitramine (Me-NENA), 2,2-diazidodiethylmalonat, (DE-DAM), 2,3-diazidopropan-1-ol (2,3-DAP), bis(1,3-diazidopropan-2-yl)malonat (1,3-TAdPM) and other similar explosives. All these substances are characterized by a number of properties derived from the results of low-temperature X-ray diffraction, infrared and Raman spectroscopy, nuclear magnetic resonance spectroscopy, elemental analysis and differential scanning calorimetry as well by the values of their sensitivity to shock, friction and electric discharges. Molecular properties of considered explosives were determined for isolated molecules and molecular units using quantum chemistry methods implemented in the Gaussian 09 computer program. The B3LYP hybrid functional and the 6-31+G(d) basis set of electron functions were used in most of performed calculations. All the geometric and energetic characteristics of these objects were calculated and the main primary mechanisms of their decomposition were determined. Their infrared and Raman spectra were calculated too. The heats of formation of the explosives were calculated using the CBS-4M method of complete basis set. All parameters of detonation waves and the equations of state for detonation products in the form of Jones-Wilkins-Lee were determined using the EXPLO5 V.6.02 program. Such calculations were performed for different initial densities of explosives and for some formulations containing these explosives as plasticizers. The calculations of exploding action of examined explosives and formulations were conducted using the ANSYS Autodyn program. Copper barriers were used for a common comparative analysis. A complete comparative analysis of obtained results was conducted and the comparison was made with similar results obtained for several classic plasticizing explosives such as glycerol trinitrate, bis(2,2-dinitropropyl)acetal and ethylene glycol bis(azidoacetate).

Nitrogen-rich salts of 3,4-bis(4-nitramino-1,2,5-oxadiazol-3-yl)-1,2,5-furoxan (BNAFF)

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Keywords: nitrogen-rich salts; energetic materials; furoxanes; furazanes.

3,4-Bis(4-amino-1,2,5-oxadiazol-3-yl)-1,2,5-furoxane (BAFF) was nitrated in 100 % HNO3 at –10 °C and then reacted with KOH to give the corresponding energetic dipotassium salt of 3,4-bis(4-nitramino-1,2,5-oxadiazol-3-yl)-1,2,5-oxydiazole-2-oxide (K2BNAFF). The neutral nitraminofuroxane compound (H2BNAFF) is unstable at room temperature and can be obtained from K2BNAFF with 2 M HCl and ether as BNAFF•Et2O. Several nitrogen-rich salts (e.g. ammonium, guanidinium, aminoguanidinium, hydrazinium and hydroxylammonium) were prepared from K2BNAFF. Few compounds were characterized by low-temperature X-ray diffraction. In addition, all compounds were analyzed by vibrational spectroscopy (IR and Raman), multinuclear (1H, 13C, 14N) NMR spectroscopy, differential scanning calorimetry (DSC) and by elemental analysis. The heats of formation for all compounds were calculated using the atomization method based on CBS-4M enthalpies. Several detonation parameters were predicted by using the EXPLO5 code (V6.03). In addition, the sensitivities of all BNAFF salts toward friction, impact and electrostatic discharge were determined according the BAM standards.

Estimation of detonation velocities for TKX-50, MAD-X1, BDNAPM, BTNPM, TKX-55 and DAAF using the Laser-induced Air Shock from Energetic Materials method

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Keywords: LASEM; TKX-50; TKX-55; MAD-X1; DAAF.

Continuing research for new energetic materials is dictated by growing requirements concerning mostly safety, environmental and performance issues. In order to fulfill those demands, many new energetic materials have been recently synthesized and characterized. Due to both safety and cost reasons, those species are initially produced on a small scale. Therefore there is a highly justified demand for laboratory-scale methods for characterizing their performance in order to determine the most promising candidates for scale-up. Laser-induced air shock from energetic materials (LASEM) is a promising new technique for estimating the detonation velocity of explosives using milligram amounts of investigated material which simultaneously provides information about the high temperature chemical reactions. Therein, LASEM has been applied to the following explosives for the first time: dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate (TKX-50), dihydroxylammonium 5,5'-bis(3-nitro-1,2,4-triazolate-1N-oxide) (MAD-X1), bis(4-amino-3,5-dinitropyrazol-1-yl)methane (BDNAPM), bis(3,4,5-trinitropyrazol-1-yl)methane (BTNPM), 5,5'-bis(2,4,6-trinitrophenyl)-2,2'-bi(1,3,4-oxadiazole) (TKX-55), and 3,3'-diamino-4,4'-azoxyfurazan (DAAF). The estimated detonation velocities for explosives being investigated were compared to calculated values from CHEETAH and EXPLO5 thermochemical codes. The LASEM results suggest that TKX-55, BDNAPM, and BTNPM have higher detonation velocities than predicted by the thermochemical codes, while the estimated detonation velocities for MAD-X1 and TKX-50 are slightly lower than those predicted.

Propellants' combustion tests of propellants with laboratory rocket motor and ballistic pendulum method

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Keywords: laboratory rocket motor (LRM); ballistic pendulum; pressure impulse; burning rate; work ability.

This paper presents new research methodology of propellants for evaluate their effectiveness for treatments associated with the intensification of oil and gas. Ballistic pendulum method is the traditional measurement of the work ability of explosives. In turn, for propellants properties testing laboratory rocket motor method is known. Using laboratory rocket motor installed in a mortar ballistic pendulum, the energetic parameters (eg., maximum pressure of the gaseous products, pressure impulse, burning rate, work ability) for selected propellants were determined.

Physical and chemical properties of the pyrotechnic composition contained in fireworks

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Keywords: fireworks; pyrotechnic composition.

The article deals with fireworks, which are primarily intended for entertainment and which may have in some case destructive potential; physical and chemical properties of some pyrotechnic composition contained in firework products and possibility of misuse of fireworks for terrorist purposes.

Additives effects on the performance of decoy flares

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Keywords: pyrotechnics; decoy flares; radiant emittance.

ADDITIVES EFFECTS ON THE PERFORMANCE OF DECOY FLARES

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ABSTRACT Pyrotechnic decoy flares are the most effective passive countermeasures for different heat seeking missiles. The advance of detectors and different operating conditions when using decoy flares forced the researcher to increase the performance of it by using different methods. One of the methods is to increases the ignition ability using different additives as C,Zr. This Additive have different effects on the performance of decoy flares as it affect both burning rate and spectral radiant emittance. Three MTV decoy flares samples were prepared with different additives e.g.(graphite and zirconium) with percentage (10%).

In this study, theoretical and experimental comparisons between all prepared decoy flare compositions were carried out. Flame temperature and burning time were measured using inframetric radiometer. Radiant emittance was calculated using a designed computer program. The result shows a high burning rate was accomplished with strong deflagration and no deformation occurs to the pellet in case of using additives.

KEY WORDS Pyrotechnics, Decoy flares, Radiant emittance,

Nomenclature

MTV Mg/Teflon/Viton

Different types of binder for decoy flare compositions

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Keywords: decoy flares; counter measures.

DIFFERENT TYPES OF BINDER FOR DECOY FLARE COMPOSITIONS Ahmed hawass, Hosam mostafa, Mohamed ismail ABSTRACT Decoy flares as a counter measures still the effective tool against different IR detectors working on different bands as (α) (1.8 - 2.5 μm) and mid wave (β) (3.5 -4.8 μm) band. Modification of the MTV compositions by using different types of binders give the chance to choice the suitable binder for suitable processing and performance of the decoy flare compositions. In this study, experimental comparisons between different MT flare compositions with different binder types (Epoxy, Shellac, Viton) were carried out. Three different compositions with different binder type and constant fuel to oxidizer ratio (30 to 65 %) was fabricated. Flame temperature and burning time were measured using inframetric radiometer. Radiant emittance was calculated using computer program. Results show that, the decoy flares based on epoxy is preferable than the other types as it have larger emittance, extended burning time(7 sec) and easily fabrication. KEY WORDS Decoy flares, counter measures.

The research of characteristics of combusting homogeneous propellants in laboratory rocket motor

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Keywords: combustion characteristics; homogeneous propellants; laboratory rocket motor (LRM).

The paper presents research results from combusting high-energy solid rocket fuels (propellants) in laboratory rocket motor (LRM). The process of combusting high-energy fuel is characterized by fast chemical reaction, which causes creating gaseous product with high pressure. The value of pressure from combusting propellants can be controlled in laboratory rocket motor by an appropriate selection of mass of the fuel and the diameter of jet. Selecting fuel which has bigger mass we can obtain bigger value of pressure as compared to choose smaller mass of fuel. The jet was replaced by solid coal cylinder. With the use of sensors there was registered a pressure inside the combustion chamber during every attempt of ignition of propellants. The aim of the paper is presentation and comparison of the pressure change graphs which were created in result of combusting high-energy materials and coal fracturing .

Ultrasound-assisted synthesis of ZnO and NiO nanoparticles and their catalytic performance on thermal decomposition of ammonium perchlorate

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Keywords: ammonium perchlorate; metal oxides; ultrasound-assisted; thermal decomposition; catalytic performance.

In this study, ZnO and NiO nanoparticles were synthesized by a simple and facile sonochemical route from zinc acetate, nickel acetate and sodium hydroxide as a precursers and calcination treatment. The utilization of ultrasound for synthesis of materials has been extensively examined over many years, and is now proven to be a powerful technique to obtain nanostructured materials. The as- prepared products were characterized by powder X-ray diffraction (XRD), field-emission scanning electron microscopy (FESEM) and studied as an efficient catalyst for thermal decomposition of ammonium perchlorate (AP). The catalytic performance of the as-prepared ZnO and NiO NPs was investigated by thermal gravimetric analysis and differential scanning calorimeter (TGA/DSC). The results showed that the addition of 4% nanosized as- prepared samples merges two exothermic peaks of AP, into one peak. The HTD peak of AP in the presence of ZnO and NiO NPs shifted downward about 120 and 105 ˚C, respectively and the total heat release (ΔH) from decomposition of AP is significantly increased to 1215.42 and 1224.33 Jg-1 in comparison with 540 Jg-1 for pure AP.

Theoretical study on thermal decomposition of 2,4-dinitroimidazole

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Keywords: theoretical study; 2,4-dinitroimidazole; thermal decomposition; rate constant.

The geometry structures of 2,4-Dinitroimidazole were calculated by density functional theory at the B3LYP/6-311G(d,p) level. The Wiberg bond indexes and NBO charges of 2,4-Dinitroimidazole molecule were analyzed by using Natural Bond Orbital theory. The thermal decomposition pathways of 2,4-DNI were studied by ab initio molecular dynamics simulations.Results showed that C-NO2 cleavage was the primary initial step in the thermal decomposition of 2,4-Dinitroimidazole. Nitro-nitrite isomerization reaction was feasible in thermodynamics but infeasible in dynamics.

An engineering approach to modeling sub-detonative events

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Keywords: explosives; thermal initiation; shock initiation; shock-to-detonation transition; SDT; deflagration-to-detonation transition; DDT; user defined subroutine; response; violence.

Shock or thermal initiation can lead to sub-detonative events such as deflagration or a burning reaction which can grow into a full-fledged steady-state detonation under certain circumstances. Shock-to-Detonation Transition (SDT) being the simplest reaction mechanism which can give rise to detonation occurs when the shock generated by a high-velocity fragment or bullet is sufficiently strong to lead to prompt shock initiation. On the other hand, the likelihood of delayed mechanisms such as Deflagration-to-Detonation Transition (DDT) occurring is very dependent on a myriad of factors such as the initial state of the explosive material, the magnitude of deformation and damage suffered by the material after stimuli and containment. If an explosive is highly confined, detonable and its diameter is greater than its failure diameter, the reaction may undergo an abrupt transition from deflagration to detonation as reaction product gases are produced leading to a rapid rise in pressure, temperature and reaction rate. To account for all the factors leading to DDT is non-trivial, and an ongoing feat for top scientists around the world today.

This work presents an engineering approach to model the transition of a low-strength compressive wave resulting from burning or a low-velocity impact to a high velocity detonation wave. The approach involves the incorporation of a user-defined subroutine in the standard hydrodynamics code ANSYS AUTODYN describing an equation of state which switches from a propellant burn model to a reactive burn model when the critical energy criterion is met. The response of an exemplary explosive will be modeled using this approach, and the results are compared qualitatively with published experimental findings. Design factors like level of confinement, venting will be considered in modeling the violence of the reaction under thermal and mechanical threats.

Synthesis and structure of high-energy polyazidopyridines

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Keywords: azides; pyridines; energetic materials; primary explosives; heats of formation.

The synthesis, structure and properties of high-energy 3,4,5-triazidopyridine-2,6-dicarbonitrile and 2,3,5,6-tetraazidopyridine-4-carbonitrile are reported.

On the mechanism of pyrolysis of (5-nitrotetrazolato-N2)pentaamminecobalt (III) perchlorate

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Keywords: pyrolysis; complexes of cobalt; anion of 5-nitrotetrazole; mass spectrometry.

Abstract. The pyrolysis of (5-nitrotetrazolato-N2)pentaammincobalt(III) perchlorate (NCP), its ligand (an anion of 5-nitrotetrazole) and the original complex - aquapentaammincobalt(III) perchlorate (APCP) have been studied by the method of mass spectrometry in order to establish details of the thermal decomposition of the light sensitive energetic material NCP. It has been shown that at 250 0C the main ligand oxidizer is changed. Outer-perchlorate ion becomes the main oxidizing agent above this temperature. It has been found that the main products of the pyrolysis of the studied compounds depend on the decomposition temperatures

Crystal structure simulation of TTTO-isomers

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Keywords: HEDM; method of atom-atom potentials; molecular electrostatic potential; TTTO; crystal structure.

Simulation of the crystal structure of two isomeric forms of TTTO - ([1,2,3,4]tetrazino[5,6-e][1,2,3,4]tetrazine-1,3,6,8-tetraoxide (1) and [1,2,3,4]tetrazino[5,6-e][1,2,3,4]tetrazine-1,3,5,7-tetraoxide (2)) was carried out. Original technique was used for approximation of the molecular electrostatic potentials (MEP) on the base of point charges obtained from ab initio calculations. The best models of isomeric molecules were further used to simulate the crystal packing of molecules within the framework of the AAP method with refined parameters of the Lennard-Jones potential ("6-12") by optimization the parameters of the unit cell and localization of the corresponding minima of the potential energy surface. Optimal crystal structure and density of TTTO-isomeric forms were determined and was shown that isomer 1 possesses the greatest density 2.03 g/cm3 (0 K) from two considered isomers.

Features of PETN explosive decomposition induced by an electron beam with the explosive-emission cathode

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Keywords: PETN; initiation; electron beam.

In this work it was investigated the PETN initiation under the joint actions of the electron beam and the low-temperature metal diode plasma of the accelerator GIN-600 (240 keV, 20 ns) with the explosive emission cathode, the critical energy density of the explosive decomposition was measured. When the energy density was equal to H ≤ 6 J/cm2 visible changes in the samples were not observed. By increasing the density in the range of H = 7 - 11 J/cm2 for samples subjected only to the electron beam action, surface damages were observed or parts of a tablet were diffused. When the actions of electrons and plasma were combined the explosion was observed with a probability of 20%. At the same time, unexploded remains of the samples were not observed in the experimental chamber. It can be concluded that under the joint effect of the plasma and electrons in the energy density range H = 9 - 11 J/cm2 there was a competition of combustion and explosion processes. The critical energy density is equal to Hcr = 14,5 J/cm2 for the electron beam and Hcr = 13,5 J/cm2 for the joint actions of electrons and plasma. It can be concluded that the plasma contribution to the Hcr is not more than 10%. When energy is equal to H ≥ 20 J/cm2 probability of the explosion is 100% for both cases. Therefore the detonation processing in the samples is mainly due to the influence of the electron beam, but the contribution of the low-temperature plasma metal to this action is negligible one.

The influence of structure of substituted azoles on the thermal decomposition rate of trinitromethyl group

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Keywords: kinetics; azoles; Arrhenius parameters; steric constants of substituents.

Kinetics and mechanism of thermal decomposition of substituted triazoles and tetrazoles, containing trinitromethyl group, are studied by manometric and photoelectrocolorimetric methods. Mass-spectrometry and chromatography are also used for analysis of decomposition products. The limiting stage activation parameters are established. It is shown that the thermal stability of trinitromethyl group is determined by the steric effect of azol. Thermal decomposition rate constant and activation energy correlate with steric constant of azole. Thermal decomposition of β-trinitroethylaminotetrazoles occurs heterolytically with the primary dissociation of C-C bond and formation of carbocation and nitroform anion.

OPTIMEX: Detonation pressure measurement using passive optical system

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Keywords: detonation pressure; shock wave; optical fiber; Optimex.

The article shows a simple method which allows determination of detonation pressure using shock velocity measurement in inert block attached to the tested explosive charge. A pressed explosive charges (95% RDX, 5% binder) were tested at a density of 1.63 g·cm 3. Nonreactive shock was tracked in various inert materials discontinuously using series of fiber optic probes and a passive light acquisition system. The detonation pressure of 24.9 GPa was then determined by impedance matching technique. The use of opaque inert materials was found to be favorable because of simple light record evaluation.

On the importance of electrostatic discharge sensitivity testing

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Keywords: explosives; sensitivity; impact; friction; electrostatic discharge.

The paper compares initiation sources involved in accidents connected with handling or manufacture of energetic materials. When a new explosive is synthesized, just an impact and friction sensitivities are often measured to describe the overall sensitivity of the sample. The same applies when a change in the production technology influences the nature of already manufactured material. The aim of this paper is to point out that the electrostatic discharge (ESD) sensitivity is not proportional to the impact or friction sensitivities and therefore must be studied separately in order to get the complete figure of the risk associated with the given material. The analysis of a large set of industrial accidents in explosives' production shows that the ESD accidents are quite common even with well-known explosives within approved production lines. Low ESD sensitivity is thus a required parameter for new energetic materials.

First attempts in cylinder expansion testing

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Keywords: cylinder expansion test; photonic Doppler velocimetry; PLX; nitromethane.

The paper deals with cylinder expansion testing of sensitized nitromethane (PLX) confined in copper and aluminium tubes. The experiments were instrumented with Photonic Doppler velocimetry (PDV) and high speed framing camera to track expansion of the tubes. The PDV velocity-time records of the cylinder wall were converted to displacement-time profiles and then a fitting procedure was employed to find pressure-volume dependence of the expanding detonation products. The results compare to those obtained using Explo5 thermochemical code as well as to the literature data. An average Gurney velocity value of 2344 ± 40 m·s-1 was found. The results obtained with aluminium tubes were slightly lower than those with copper tubes. High speed photographs showed that there was no premature breakage of the tubes, although common materials were used.

Determination of explosion parameters of dust clouds depending on the vertical location of igniter

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Keywords: explosion characteristics; maximum explosion pressure; vertical position.

The article deals with the study of the effect of vertical location of igniter in the explosion chamber to the maximum explosion pressure. The measurements were carried out according to STN EN 14034-1+A1:2011 Determination of explosion characteristics of dust clouds. Part 1: Determination of the maximum explosion pressure p_{max} of dust clouds. A modified KV 150-M2 chamber was used to measure the monitored characteristics. The beech dust cloud in the chamber is achieved mechanically by high pressure air flow. The sample is ignited by nitrocellulose igniter after dispersing of the sample in explosion chamber. Immediate initiation of nitrocellulose is achieved by the voltage value which is supplied to the resistance wire. Ignition energy of nitrocellulose used in igniter is 2x5 kJ. Determination of explosion parameters of beech dust clouds depending on the vertical location of igniter was performed in 7 positions. The maximum value of the pressure 6,58 bar was reached at the position 12 cm above dispersing system.

Prediction of thermal properties for energetic material using isothermal analysis

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Keywords: energetic materials; thermal properties; DSC.

Thermal properties are most important characters in the field of energetic materials. Many tools and methods are developed for analysis and evaluation of energetic materials. Differential Scanning Calorimetry(DSC) is a typical method for thermal analysis not only for common chemicals but also energetic materials. Because energetic materials generally release certain amount of heat when they are decomposed, DSC is used frequently to evaluate thermal properties of energetic materials. In the DSC measurements, sometimes thermodynamic change such as melting interfere kinetic evaluation of materials. So isothermal method is often performed to avoid thermodynamic issues. In this research, we used AKTS thermokinetic program to predict thermal properties. Here in, we report prediction of properties for energetic materials using AKTS program through isothermal DSC measurements.

Investigating the transport of gases and decomposition pathways in plasticized nitrocellulose materials

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Keywords: nitrocellulose; plasticiser; degradation.

Nitrocellulose is a complex energetic polymer widely used throughout the propellants industry, with explosive properties once the nitrogen content is above 12.6 %. During the storage of nitrocellulose, degradation occurs through a series of steps. As a result, a number of gases are produced including NO_2, which is thought to lead to autocatalysis of nitrocellulose decomposition. Stabilisers are often added to nitrocellulose propellant formulations, which absorb these decomposition products and plasticisers are added to satisfy mechanical properties and safety requirements. The transport and solubility of gases in plasticised nitrocellulose will be investigated. The dominant degradation and autocatalytic processes of nitrocellulose will be examined using density functional theory. Preliminary studies will investigate the proposed mechanisms for homolytic fission, intramolecular HNO_2 elimination and acid hydrolysis.

The effect of multi-modal particle system on shock sensitivity of highly filled pressable PBX

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Keywords: multi-modal particle system; shock sensitivity; pressable PBX.

In pressable PBX, densification in compaction occurs by rearrangement and deformation of explosive particles. If the brittle explosive particles are compressed till particle fraction is higher than theoretical random close packing fraction(RCPF), bigger particles of them should be fractured to fill the void. Multi-modal particle system can be used to get high density without particle fracture increasing RCPF. Fracture surface is assumed to be origin of hot spot and make the PBXs sensitive to external stimulus. In this study, multi-modal particle system was introduced for the decrease in possibility of particle fracture during compaction expecting decrease in shock sensitivity of highly filled pressable PBX. The experimental result showed the trimodal particle system had low sensitivity and high density, compared to bimodal particle system.

Dispersion of condensed combustion products of solid composite propellants based on Zr or its hydride

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Keywords: Zirconium; combustion; propellants; combustion products dispersion.

The degree of dispersion of condensed combustion products of solid composite propellants (SCP)containing zirconium or its hydride is studied. It was shown that in the case of Zr-containing SCP the average size of the condensed combustion products (zirconium dioxide) is close to the average size of the initial zirconium powder, while in the case of ZrH2- containing SCP it is considerably larger than the size of the initial ZrH2. The reason of this phenomenon is under consideration

Thermochemical and energetic properties of DNTF and DNFF

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Keywords: bis(4′-nitrofurazan-3′-yl)furazan; 3,4-bis(4′-nitrofurazan-3′-yl)furoxan; enthalphy of formation; crystal structure; solid composite propellants; specific impulse.

Bis(4′-nitrofurazan-3′-yl)furazan (DNTF) and 3,4-bis(4′-nitrofurazan-3′-yl)furoxan (DNFF) have been investigated as potential compounds of solid composite propellants. The experimental values of their enthalpies of combustion and standard enthalpies of formation have been obtained. Δ Hf values are 662.0 ± 2.4 and 635.2 ± 1.2 kJ/mol respectively for DNTF and DNFF. X-Ray analysis showed that DNTF crystals are orthorhombic (space group P212121), at room temperature a= 7.1470(3); b= 9.7901(5); c= 15.2766(7) Å; $\alpha=\beta=\gamma=90^\circ$; $\rho=1.84$ g/cm3. DNFF crystals are orthorhombic (space group P212121), at room temperature a= 6.7887(6); b= 10.8072(7); c= 15.2355(16) Å; $\alpha=\beta=\gamma=90^\circ$; $\rho=1.855$ g/cm3. I was shown that both DNTF and DNFF are low effective with hydrocarbon binders, but with active binder it is rather simple to reach specific impulse Isp (at Pc:Pa=40:1) equal to 254.5 s at $\rho=1.78$ g/cm3 in metal-free formulations basing on DNTF, and Isp=258 s at $\rho=1.80$ g/cm3 in metal-free formulations basing on DNFF

Bimolecular srystal CL-20*7H-tris([1,2,5]oxadiazole)[3,4-b:3',4'-d:3",4"-f]azepine; its standard enthalpy of formation and thermal stability

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Keywords: CL-20; bimolecular crystals; enthalphy of formation; thermal stability.

The standard enthalpies of combustion and enthalphy of formation (EF) of 7H-tris([1,2,5]oxa-diazole)[3,4-b:3',4'-d:3",4"-f]azepine (HTFAZ), its bimolecular crystal (BMC) with CL-20 γ-polymorphy in molar ratio 1:1, and the γ-polymorph of CL-20 itself have been experimentally determined. It has been established that the difference between EF of BMC 1007.5±6.7 kJ/mol and EF of the equimolecular mechanical mixture γ -CL-20 and HTFAZ (995.9 kJ/mol) differ by no more than 12 kJ/mol, that is a level of a measurement deviation. Quantum-chemical calculations have shown that BMC does not possess any additional energy as compared to the total energy of the initial isolated crystals HTFAZ and γ -CL-20 and the value of the standard EF can be considered to a first approximation as the sum of the EFs of the original crystals. The difference of about 4.2 kJ/mol does not affect the energy performance of compositions. It has been established that during thermal decomposition of BMC γ -CL-20 with HTFAZ the main contribution to the heat release rate makes the decomposition of CL-20. HTFAZ presented in the BMC, even inhibits the thermal decomposition of CL-20. This phenomenon lets to increase the shelf life of the BMC compared to the shelf life of the initial CL-20.

Theoretical simulation of the glass transition temperature and mechanical properties of modified Glycidyl Azide Polymer

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Zong-kai Wu, Yao Shu, Xiao-chuan Wang, Xiao-yong Ding

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Keywords: GAP; MD simulations; glass transition temperature; mechanical property.

Molecular dynamics (MD) simulations were carried out to study the glass transition temperature and mechanical properties of glycidyl azide polymer (GAP) that are widely used in propellants and explosives as an energetic binder. Other three polymers derived from GAP with different side groups were also designed and simulated under the COMPASS forcefeild, the ensembles of constant particle number, volume, temperature (NVT) and constant particle number, pressure, temperature (NPT). It was found that the density of polymers changed regularly along with the decrease of temperature and the transition occurred at the Tg point. The simulation results showed that the introduction of –NH2 and –NO2 made important contribution on reducing the Tg of polymers, and the underlying mechanism was discussed. Moreover, several mechanical properties of four pure polymer systems were calculated, such as Young's modulus, shear modulus, bulk modulus and Poisson's ratio, etc. The calculated results revealed that the single introduction of –NO2 increased the mechanical performance index more obviously than other two polymers. Overall, this investigation firstly studied a new method to modify GAP to improve its mechanical properties at low temperature, and provided some guidance to the modification of GAP via changing substituent groups of side chain.

Hydrogen peroxide - based explosive formulation to eliminate nitrogen oxide fumes in detonation process

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Keywords: hydrogen peroxide; ammonium nitrate; nitrogen oxide fumes; detonation velocity.

This paper describes preliminary work which was conducted to create a novel formulation of explosive which eliminates post - blast nitrogen oxide fumes (NOx), as a direct product of the detonation process. During the burning reaction nitrogen oxides (NO, NO2) are produced as a result of using bulk ammonium nitrate (AN) – based commercial explosives. Exposure to this toxic gases can cause a negative effects on the health and safety of the exposed persons and surrounding environment. The aim of this study was to substitute the use of AN with hydrogen peroxide (HP) as the main oxidizing agent to minimize the NOx fume risk. The main objective of this work was to measure the velocity of detonation (VoD) of the samples at different diameters, densities and void sensitization techniques for HP/fuel – based explosive mixtures.

On the partial oxidation of 3,4–bis(4’-aminofurazanyl)furazan (ATF) and its N-oxide (AFF)

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Technology (Technical University)

Keywords: heterocyclic energetic compounds; aminofurazan; oxidation; nitrofurazan.

Using traditional oxidizing mixtures based on H2O2 and H2SO4 in the presence of ammonium persulfate was demonstrated to be capable of quenching the oxidation of 3,4 –bis(4’-aminofurazanyl)furazan (ATF) and its N-oxide (AFF) at the stage of monoaminonitro derivatives ANTF and ANFF. The optimum reaction conditions which enable synthesizing 3-(4’-ami¬ nofurazanyl)-4-(3’-nitrofurazanyl)furazan (ANTF) and 3-(4’-amino- furazanyl)-4-(3’-nitrofurazanyl)furoxan (ANFF) in 40-50% yield were worked out.

Quantum chemical study of the mechanism of C-nitroimidazo[4,5-e]benzo[1,2- c;3,4- c']difuroxane formation

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Keywords: furoxanes; DFT; computer simulation.

The possible mechanisms of nitration reaction of imidazo[4,5-e]benzo[1,2-c;3,4- c']difuroxane have been investigated using the quantum chemistry methods. The energetically more preferable pathway of synthesis for the new high energetic compound C-nitroimidazo[4,5-e]benzo[1,2-c;3,4-c']difuroxane has been found out. The synthesis of the target compound has been made in accordance with the proposed mechanism.your abstract here. Use about 300 words.

Numerical and software solution in JAVA for interior ballistics problem of smokeless powders

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Keywords: interior ballistics; smokeless powders; Runge-Kutta; Drozdov; JAVA.

Basic problem of internal ballistics is determination of laws of gases development and projectile motion in gun barrel. To solve the problem, it is necessary to develop a theory ie. to define dependencies between characteristic values. After setting-up the theory, explicit expressions are obtained which create system of internal ballistics equations. Solving of given system can be done by using analytical (Drozdov) or numerical (Runge-Kutta) methods.
 The method of Drozdov is used for guns which use only one type of smokeless powder. These include cannons, howitzers and all types of small arms.
 The Runge-Kutta method is used for calculations for just one type of powder. System of equations is transformed in such way that differential equations are given in special form and then integrated by numerical method.
 Based on mathematical models, a software is developed in JAVA for internal ballistics calculations. Software solves problem for single and multi-hole cylinder, compact cylinder, cross, spheric and hexagon powder grains, and also for flakes and strips. Results are given as explicit values (pressure, projectile velocity etc.) and in graphic form.

Getting mercaptobenzothiazole derivatives on the basis of ferrocene.

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Keywords: diethyl ether; ethanol; ferrocene; ferrocenylbutanetrion; mercaptobenthiazole.

Getting mercaptobenthiazole derivatives on basis of ferrocene. The interaction of 1-ferrocenyl-1,3-butane diol and 1,1'-ferrotsendiildibutan-1,3-diol with mercaptobenzothiazole . Characteristics and spectral properties of the mercaptobenthiazole derivatives of 1-ferrocenyl-1,3-butane diol and 1,1'-ferrotsendiildibutan-1,3-diol Keywords: diethyl ether; ethanol; ferrocene; ferrocenylbutanetrion; mercaptobenthiazole.

Photochemical initiation of PETN doped by organic carbonyl initiators

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Keywords: photoinitiators; laser initiation; PETN.

The possibility of controlling the threshold of photostimulated initiation of explosive decomposition reaction of energetic materials by the use of a photoinitiator was showed. 9,10-Phenanthrenequinone (PQ) used as the photoinitiator (that is commonly used as a photoinduced hydrogen abstracting agent) in pentaerythritol tetranitrate matrix (energetic material). Optical spectra of the obtained composite material, and its laser initiation threshold by radiation of wavelength 532 nm are determined. It showed a marked increase in sensitivity by adding the photoinitiator. The threshold of laser initiation of composite PETN-PQ 0.2%wt. is about 2 times lower than for pure PETN. DFT modeling shows noticeably facilitation the decomposition reaction.

3,3-bis(azidomethyl)oxetane and 3-azidomethyl-3-methyloxetane copolymerisation catalyzed by trialkylaluminium catalyst

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Keywords: 3,3-bis(azidomethyl)oxetane; 3-azidomethyl-3-methyloxetane; cationic ring opening polymerisation (CROP); copolymer.

The article presents the results of research of synthesis copolymers azidomethyl-substituted oxetanes. AMMO-BAMO copolymers have been synthesized with different amount of monomer AMMO units in presence of catalyst – trialkylaluminum/water. Copolymers were investigated by differential scanning calorimetry (DSC), viscometry, elemental analysis. Mechanical and physical characteristics at break of a samples were received.

Nitrocellulose and stabilizers: DFT calculations of bond dissociation and reactions

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Keywords: nitrocellulose; stabilizer; DFT.

The reaction pathways of nitrocellulose degradation and stabilisation are still a topic of current research activities. Experimentally, chain scission, analysis of gaseous products and evolved reaction heats can be measured. Apart from established facts such as the O-NO2 bond being the weakest and effects of moisture, the reaction pathway remains mostly unknown.

In this contribution, first steps of quantum-mechanical calculations are shown: Starting from a semi-amorphous nitrocellulose bulk, with the goal to calculate thermodynamic quantities of degradation reactions.

In order to generate a nitrocellulose simulation model (NC simulate), cellulose is nitrated by simple insertion of nitrate ester functionalities into a crystal supercell. The resulting structure is energetically highly unfavorable because of the comparably bulky –ONO2 groups. It is relaxed by a molecular dynamics simulation, which uses classical forcefields as COMPASS II from Materials Studio from Accelrys, now Biovia. The resulting structure shows a partially amorphous structure: Each single nitrocellulose chain arranges in a helical twisted form, and several chains are arranged in a hexagonal pattern.

From this pattern, representative single glucopyranose rings are identified and subjected to density functional theory (DFT) calculations using DMol3 from Materials Studio. (BLYP functional, and basis set similar to 6-31G* of Gaussian). Dissociation energies and enthalpies are calculated. The same procedure is applied to stabilizers such as diphenylamine.

Although the applied functional and basis sets are rather coarse, results show good agreement with experimental values for bond dissociation energies and enthalpies.

Effect of the particle size distribution of solid fillers on the mechanical properties of composite solid rocket propellant used with RAP application.

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Keywords: rocket assisted projectiles; composite solid rocket propellant.

Evidence suggests that rocket assisted projectiles (RAP) is among the most important factors for increasing the velocity of the artillery projectile and consequently the range. To date, few studies concerned with the effect of the percentage and the particle size distribution of the solid fillers on the mechanical properties of composite solid rocket propellant used with RAP application. Experimental testing for different prepared samples including mechanical properties carried out using (SEM) apparatus model MIRA3 TESCAN and universal test machine model Zwick Z050. Results showed that increasing fine to course ratio of the solid filler (22/78 to 35/65) increases tensile modulus, elongation and tensile strength, by [7.8% - 5.3% - 62%] respectively.

KEYWORDS Rocket Assisted Projectiles, Composite Solid Rocket Propellant.

Metal bistetrazolates as catalysts for ammonium perchlorate decomposition and combustion

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Keywords: ammonium perchlorate; catalyst; decomposition; combustion; bistetrazolates.

Ammonium perchlorate (AP) is widely used as an oxidizer in energetic systems, and the possibility to tailor its reaction rate and decomposition temperature by the cata-lyst addition is crucial for obtaining the desired parameters of AP-fuel mixtures. Met-al bistetrazolates comprise the high-nitrogen containing tetrazole anion with the met-al cation. During the decomposition of these salts metal particles are expected to be formed, being, according to the literature, the effective catalytic agents for AP. Here we explore catalytic abilities of bistetrazole compositions with different metals, viz., Cu, Ni, and Mn. Thermal analysis study reveals the shift of the AP exothermic high-temperature decomposition peak to the lower temperatures, proving the catalytic ac-tivity of all the investigated metal bistetrazolates. However, the burning rate of am-monium perchlorate monopropellant with 5% addition of various metal bistetrazo-lates is more complex and exhibits the increase for copper bistetrazolates only, which enhances the burning rate in more than 3 times within 2-10 MPa pressure range. On the contrary, manganese bistetrazolate even decreases the AP burning rate, appar-ently due to the crystallized water within the molecule. The results show that the com-bination of the high-nitrogen containing molecular structure with the copper cation can be successfully used as combustion catalyst for AP-fuel formulations.

Insensitive melt cast explosive compositions containing N,N-diethyl-2,4-dinitroaniline

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Keywords: melt cast composition; N,N-diethyl-2,4-dinitroaniline; TNT; Composition B.

In this paper, some results of experimental tests of melt cast compositions containing N,N-diethyl-2,4-dinitroaniline (DEDNA) are described. This research work was carried out in order to compare parameters of compositions DEDNA / TNT and DEDNA / RDX with Composition B. In order to obtain explosive compositions, DEDNA was mixed with hexogen (RDX) or 2,4,6-trinitrotoluene (TNT). The measurement results of sensitivity to mechanical stimuli, detonation velocity and thermochemical parameters like heat of combustion are presented. On the basis of the results it was found that, the addition of DEDNA decreases the impact sensitivity of the compositions, whereas the melting point of the mixtures with TNT is decreased.

Effects of TNT contaminants soil on the vegetation at an explosive range by probing UPLC qTOF MS analytical methods

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Keywords: UPLC qTOF MS; metabolites; 2,4,6 trinitrotoluene; detection; soil.

Three trees species (Wild olive, Stinkwood and Cape Holy) and one shrubs species (Dovyalis caffra) were each potted in 20 litre pots and then populated at CSIR explosive range. This was established in order to evaluate the effect of TNT-contaminated soil on vegetation. TNT contamination was established by dissolving flake TNT in acetone at various concentrations per kilogram soil. One pot for every species was left uncontaminated as control elements. The establishment of the population was completed in July 2013. A set of 16 samples, four contaminated, four uncontaminated aerial parts and their corresponding soils, were collected. These were processed and then subjected to solid phase extraction method to isolate target organic analytes of interests. A laboratory analytical methods was applied and it relies on ultra-performance liquid chromatography coupled to quadrupole time-of-flight mass spectrometry (UPLC-qTOF MS). For the UPLC-qTOF MS a gradient for the mobile phase was found which allowed the separation of the TNT and/or its residues in soil as well as other plant metabolites found in the aerial parts of the vegetation. This method allowed one to identify and quantify major changes caused by TNT contaminated soil on vegetation. The qTOF-MS was also operated under multiple reaction monitoring(MRM) mode using the electrospray ionization(ESI)technique with positive ion polarity.A clear comparison of profiles was achieved and proving the uptake of TNT by the plants.

A convenient laboratory-scale preparation of dinitrogen pentoxide (N2O5)

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Keywords: dinitrogen pentoxide; N2O5; nitration; HEDM; energetic materials.

Dinitrogen Pentoxide is a versatile reagent for the nitration of many substrates to both known and novel energetic systems. This paper details the lab scale preparation of this material using commonly-available equipment and reagents in any chemical laboratory in high purity.

Influence of accelerated ageing on thermo-mechanical properties of selected homogenous solid rocket propellants

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Keywords: accelerated ageing; DMA; DSC; TG; homogeneous propellants.

The thermo-mechanical properties of solid rocket propellants have a significant impact on the proper function of rocket motors. During use and long-term storage the properties of rocket propellants are changing, due to chemical and mechanical influences such as thermal reactions, oxidation reactions or vibrations. They can cause changes due to ageing processes of rocket motor, and in the worst case even make its accidental explosion. It's important to investigate as many thermal and mechanical properties of solid rocket propellants as possible. Dynamic Mechanical Analysis (DMA) is an effective and safe method to investigate mechanical properties of rocket propellants. This method allows to get a large amount of information about the material during a single measurement. It is possible to determine such parameters as: dynamic storage modulus (E'), dynamic loss modulus (E"), the damping factor (tan δ) and glass transition temperature (Tg). The most commonly used thermal methods to investigate the properties of solid rocket propellants is differential scanning calorimetry (DSC) and thermogravimetry (TG). The most sensitive parameters in DSC and TG curves are: heat of reaction, maximum heat flow rate, specific temperatures and mass loss at a given time. Thermal analysis is useful in determination of kinetic parameters of thermally decomposed explosives, which are significant from the point of view of safety while operating warfare agents. The parameters such as activation energy, Arrhenius factor and reaction rate constant were determined. Kissinger and Ozawa methods were applied in kinetic calculations. Mechanical properties investigation is carried out according to STANAG 4540 while thermal properties investigation is carried out according to STANAG 4515. Chosen samples of solid rocket fuels have been aged by two methods: multi-temperature accelerated ageing and according to ageing procedure proposed in AOP-48.

Coarse-grained molecular dynamics strategy on the structural change of energetic crystal: a case of α-RDX crystal against shock

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Keywords: coarse-grained molecular dynamics; alpha-RDX; mechanical property; shock; dislocation.

The meso-scale structural change of energetic crystal against shock is of significance on the mechanical and detonation properties of energetic materials. In our study, a typical energetic α-RDX crystal under shock loading was investigated using coarse-grained molecular dynamics (CG-MD) simulations, and the temperature field, pressure field, pore evaluation and shock front for both perfect and defected models were analyzed. The results show that the planet shock loading can obviously change the meso-structure of RDX crystal, plastic deformation and dislocation occur as the shock wave pass; the temperature field change with the pressure field; the void can obviously intensify the structural change, high temperature, stress, deformation and dislocation appear around the void under shock, leading to the forming of hot spots. The above show that shock loading can significantly make the structural change of RDX crystal which may leading to the detonation, and the control of voids inside the crystal is of importance on the safety of the energetic materials.

Well-known methods for non well-known compounds: the high-energetic mesoionic cores

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Keywords: quantum chemical calculations; mesoionic forms; enthalphy of formation; oxatriazoles; tetrazoles; novel high-energetic materials.

The structure of the novel compounds (mesoionic 1,2,3,4-oxatriazoles and 1,2,3,4- tetrazoles) have been calculated using ab initio quantum chemistry. Some physical chemical characteristics have been estimated. The prospectivity of these compounds as high-energetic materials was proved.

Ionic derivatives of 5,5’-(hydrazine-1,2-diyl)bis[1H-tetrazole] as new explosives

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Keywords: 5,5’-(hydrazine-1,2-diyl)bis[1H-tetrazole]; HBT; explosives.

The aim of this work was to obtain new explosive materials which could be used for military purposes. We successfully synthesized ionic derivatives of 5,5’-(hydrazine-1,2-diyl)bis[1H-tetrazole] with high yield and purity. New materials were tested with nuclear magnetic resonance. Thermal properties were examined by differential thermal analysis and thermogravimetry. Purity of the compounds was deducted from its elemental analyses. We also measured sensitivity to impact and friction stimuli.

New explosive ionic compounds based on 5,5'-azotetrazole

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Keywords: azotetrazole; explosives.

Derivatives of tetrazole form interesting group of high nitrogen materials. In this work we successfully obtained ionic derivatives of 5,5'-azotetrazole. The compounds were synthesized with high yield and purity in aqueous environment. Products were characterized with spectroscopic methods such as multinuclear magnetic resonance (1H, 13C NMR). Composition was confirmed with elemental analysis. Sensitivity to friction and impact were determined according to BAM standards. Thermal properties were measured with differential thermal analysis (DTA) and thermogravimetry (TG).

Energetic nitrate esters based on tris(hydroxymethyl)aminomethane (TRIS)

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Keywords: nitrate ester; TRIS; energetic materials; specific impulse; crystal structure.

Based on the promising performance data of N,N‘-bis(tris(nitratomethyl)methyl)oxamide, a variety of new energetic compounds were synthesized with the tris(hydroxymethyl)aminomethane (TRIS) moiety as building block. The new nitrate esters were fully characterized, including multinuclear NMR spectroscopy, vibrational analysis, differential scanning calorimetry and elemental analysis. The structure of each compound was confirmed using single crystal X-ray diffraction. The energies of formation were calculated with the GAUSSIAN program package and the detonation parameters were predicted using the EXPLO5 computer code. Their performance data were compared to the well-known nitrate ester PETN.

Physico-chemical properties and combustion behavior of low-melting oxygen-rich energetic pyrazoles

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Keywords: thermal decomposition; combustion; nitropyrazole.

At present time highly energetic pyrazoles containing oxygen-rich trinitromethyl or dinitromethyl groups were synthesized. To make effective use of these compounds is necessary to know their basic properties that determine their performance and stability. Accordingly, the present study was devoted to the study of thermal properties and combustion of two isomeric dinitropyrazoles, N-trinitrometyl-3,4-nitropyrazole and N-trinitromethyl-3,5-nitropyrazole and N-fluorodinitrometyl-3,5-dinitropyrazole and N-(difluoroamino)dinitromethyl-3,5-nitropyrazole.

Thermal decomposition of nitrogen-rich energetic compounds: new insights from high-level ab-initio calculations

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Keywords: energetic materials; nitrogen-rich hererocycles; thermal decomposition; activation barriers; CCSD(T)-F12 calculations.

Azobis tetrazole and triazole derivatives containing long catenated nitrogen atom chains are of great interest as promising green energetic materials. Kinetics and mechanism of the primary decomposition reactions of azobistriazole, azobistetrazole, and the methyl and nitro derivatives of the latter were studied theoretically using highly accurate CCSD(T) F12b/VDZ-F12 level of theory. Similarly to parent triazole and tetrazole, all azobis species under study decompose via the ring opening followed by the elimination of N2. In the case of azobistetrazole derivatives, the calculated activation barriers of de-composition are 26-34 kcal/mol, which is notably low from that of tetrazole (40 kcal/mol). This fact agrees well with the observed low thermal stability and high impact sensitivity of these species. In contrast, the activation barrier of azobistriazole decomposition was calculated to be 46 kcal/mol, which is close to that of triazole.

A systematic design strategy for bistetrazole low sensitivity high energy density materials (HDEMs): Combining N-oxidation, hydroxylammonium salt formation, aromaticity and resonance theory

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Keywords: TKX-50 derivatives; N-oxides; DFT; Detonation property; AdNDP theory.

Several molecular design strategies, such as N-oxidation, hydroxylammonium salt formation, aromaticity theory, resonance theory and conjugation system, have been used with quantum chemistry methods' help to develop bistetrazole derivative for screening out an effective explosive design strategy and high performance and low sensitivity HEDMs at the same time. The structures and properties have been evaluated and analyzed with quantum chemistry calculations and thermodynamics methods under DFT B3LYP 6-31++g (d, p) level, and some of these designed compounds exhibit outstanding performance as promising powerful and insensitive energetic compounds. Furthermore, the Adaptive natural density partitioning (AdNDP) method and resonance theory have been employed to analyze the stability of the title compounds. Among these designed molecules, Dihydroxylammonium 1H,1'H-[5,5'-bitetrazole] 3,3'-dioxide (HABTNO) and dihydroxylammonium 1,1'-diolate-1H,1'H-[5,5'-bitetrazole] 3,3'-dioxide (TKXO-50) have shown perfect detonation properties. The detonation velocity and detonation pressure of TKXO-50, in order, are 10938m/s and 55.1GPa, which are even better than those of CL-20 while its impact sensitivity (h50, 38cm) is far more stable than CL-20. These results indicate that this systematic design strategy for bistetrazole derivatives is effective and reliable which can design novel explosives with high energetic properties and low sensitivity.

Production of spherical ternary energetic composites by crystallization

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Keywords: ammonium perchlorate; RDX; thermal decomposition; crystallization.

In the present work, the spherical composites of Al/RDX/AP were prepared by drowning-out/agglomeration (D/A) process. The onset temperature of thermal decomposition of composites by the D/A process was found to decrease in comparison with that of by physical mixing, and furthermore their thermal stability was relatively enhanced. In the first decomposition of AP, Prout-Tompkins model appears to describe well the thermal decomposition of both composites by physical mixing and the D/A process. However, in the second decomposition of AP, the decomposition mechanism of composites by physical mixing was shown to be described by the zero-order model and that by the D/A process was found to be explained by the contracting volume model.

The study of the thermal and ballistic properties of SMX

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Keywords: SMX; nitroglycerine; nitrate ester; burning rate; DSC; decomposition.

Combustion of SMX and possibilities of its catalysis have been studied. It has been established that there is a burning rate increase is observed when we replace nitroglycerine on SMX. With use of scanning electron microscope is shown that SMX powder particles have pronounced crystal faceting. The thermal stability has been studied with use of differential scanning calorimetry. The decomposition rate constant equation has been found. It was shown that at isothermal conditions (90 °C) the amount of decomposed SMX is 0,8% mass for 60 minutes. With use of thermal gravimetrical analysis it was shown that there are two different processes is taken place when SMX is heated – decomposition and evaporation, herewith SMX is evaporate faster than decompose.

Influence of polyacrylamide and stearic acid on crystal growth of RDX Part II: Sensitivity testing of RDX in Composition B

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Keywords: RDX; crystallization; polyacrylamide; stearic acid; GAP.

Cooling and antisolvent crystallizations of RDX from acetone solutions were performed. In the case of addition of stearic acid during cooling crystallization more spherical and less impact sensitive crystals were obtained. From prepared RDX samples Composition B charges for GAP test and other sensitivity test methods were casted. Stearic acid strongly decreases nucleation rate and causes formation of less internal defect crystals. Material obtained by cooling crystallization showed reduced sensitivity characteristics, similar to RS-Dyno Nobel RDX. In the case of polyacrylamide addition, high bulk density RDX materials resulted. Its sensitivity to shock wave was relatively high, making it suitable material for blasting caps, sheet explosives and paste explosives, where propagation of blast wave in small diameter is required.

Prediction of explosives characteristics and optimization of the chemical composition of explosives

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Keywords: structure of compounds; enthalphy of formation; molecular crystal density; velocity of detonation; impact sensitivity; electrical spark sensitivity.

Computational methods, based on a large number of experimental data on the study of the enthalpy of formation and density of molecular crystals, have been used for the development of design schemes to evaluate of the basic characteristics of high-energy materials and explosives. It is shown the influence of the certain types of atoms on the density and the enthalpy, and, consequently, on the energy capabilities of explosives. It is noted, that the calculation of pressure, detonation velocity, the heat of explosion and some other explosion performances does not demand such complex schemas, as for calculations of the density and the enthalpy of formation, and rather a small set of parameters is required to estimate the safety factors. All of these design parameters are the basis for the evaluation of physical and chemical characteristics of energetic compositions and these characteristics are represented by numerical values and graphically in the study.

Explosives with addition of organic waste

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Keywords: blasting; emulsion explosives; organic waste.

Detonability of low density explosive, based on emulsion explosive that has reduced density, and has been sensitized by adding expanded polystyrene and organic waste such as milled hay, has been determined by measuring the velocity of detonation. Different types of explosive mixtures were tested, and their work ability was deter-mined, to find an optimal ratio of low density emulsion explosive and organic waste.

Synthesis, characterization and thermal properties of 5-(4-azidofurazan-3-yl)-1H-tetrazol-1-ol

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Keywords: azidofurazan; nitrofurazan; 1,2,5-oxadiazole; 1,2,4-oxadiazole; tetrazoles; amidrazone.

This report presents an accessible synthetic route for preparation of 5-(4-azidofurazan-3-yl)-1H-tetrazol-1-ol (AzFTol) and its ammonium salt (AzFTol•NH3) from synthetically available amidoxime of 4-aminofurazan-3-carboxylic acid. The title energetic compounds were characterized by IR, 1H, 13C, 15N NMR spectroscopy, X-ray diffraction analysis and differential scanning calorimetry. The crystal of AzFTol•H2O belongs to monoclinic syn-gony, space group is P21/c with a = 10.0019(14), b = 6.2195(7), c = 13.5749(18) Å, α = 90, β = 107.701o, γ = 90, V = 804.48(19) Å3, Z = 4, d = 1.760 g•cm-3 (monohydrate at 100K), m = 0.154 mm-1. The decomposition point is 187oC. The crystal of AzFTol•NH3 be-longs to ortorombic syngony, space group is P21/21/21 with a = 4.7397(3), b = 12.0960(6), c = 13.9889(6) Å, α = 90, β = 90o, γ = 90, V = 802.01(7) Å3, Z = 4, d = 1.757 g•cm-3 (monohydrate at 100K), m = 0.149 mm-1. The decomposition point is 179oC.

Synthesis and X-ray crystal structure of TNC (1,3,6,8-tetranitrocarbazole)

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Keywords: carbazole; nitrocompounds; nitration reactions; tetranitrocarbazole; TNC; synthesis; spectra; LC-MS analysis; crystal structure; X-ray diffraction; density; HEM.

1,3,6,8-Tetranitrocarbazole (TNC) (C13H5N5O8) found its application in millitary practice in some pyrotechnic compositions for the illuminating and firring material formulations. In this work TNC has been synthesized by two different nitration methods (yields: 62 and 58.9%). The structures of nitration reaction products were confirmed by spectral methods. It has been found for the first time, that carbazole nitration to TNC was accompanied by formation of its minor product, pentanitroderivative, (MW=392, 1,2,3,6,8-pentanitrocarbazole), which, most probably, formed in the reaction by nitration of other (minor) TNC isomer, 1,2,6,8-TNC. The concentrations of pentanitro product, obtained by different nitration methods, were defined to be equal to 4-10%. The monocrystal of pure 1,3,6,8-TNC was grown from its solution in nitromethane and was used for the detailed X-ray structure determination. It was found, that TNC crystallizes in monoclinic crystal system, space group P21/c, specific crystal density: 1.765 (calc., at -100°C) or 1.73 (measured by picnometer at 20°C). Interestingly, this TNC density value is superior in comparison with TNT (1.654 g/cm3). The main properties of TNC: formula weight: 347.21; melting point: 296°C; flash point: 350°C; solubility in water: practically insoluble; heat of formation: -18.9 kJ/ mol and density at room temperature: 1.73 g/cm.

Energetic polyurethane elastomers based on beta-cyclodextrin partial nitrates and various energetic oligodiols: synthesis and investigation of properties

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Keywords: partial beta-cyclodextrin nitrates; polyurethane elastomers; synthesis; properties.

Investigations aimed at determination of the possibility of using cyclodextrin nitrates and their derivatives as energetic components of propellants and explosives have been carried out for more than 20 years. In the available literature there can be found a description of several attempts of cyclodextrin nitrates utilization in a pure form, as inclusion complexes with different energetic compositions and as polimers. Methods of synthesis of cyclodextrin nitrates polymers described in literature can be reduced to a synthesis of cyclodextrin polymer followed by its nitration. Branched cyclodextrin polymers can be obtained by interaction with various diisocyanates. In this case a cyclodextrin molecule is included in each link of the polymer chain. However, a polymer consisting only of cyclodextrin links does not behave as an elastomer. To obtain elastomers based on cyclodextrin nitrates it is required to copolymerize them with compounds which provide the polymer chain with the flexibility needed. Energetic polyurethane elastomers based on partial beta-cyclodextrin nitrates and various energetic oligodiols are synthesized. Oligomers of the following compounds were used as energetic oligodiols: 3,3-bis(azidomethyl)oxetane, 3-azidomethyl-3-methyloxetane, glycidyl azide and glycidyl nitrate. The energetic oligodiols were used as linear blocks, and partial cyclodextrin nitrates were used as branching agents. The structure of the synthesized energetic polyurethane elastomers was determined by IR-spectroscopy, NMR spectrometry and gel permeation chromatography. Combustion enthalpy was determined and formation enthalpy was calculated from it. Also thermal, physico-mechanical and physico-chemical properties of the synthesized energetic polyurethane elastomers were studied. The work was supported by Russian Foundation for Basic Research (grant 16-29-01041 ofr-m).

Assessment of weapon-ammunitions systems in forensic ballistic

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Keywords: forensic; ballistic; gun propellants.

This paper presents theoretical predictions and experimental tests made in order to assess the system weapon-ammunition for small arms of interest in forensic science. A dedicated test configuration was designed aiming to evaluate the correlation between average pressures of gaseous products, gunpowder loading density, powder manufacturing process, weight of the propellant charge, bullet discharge force, forcing cone, bore enlargement, muzzle velocity. Interior ballistic parameters for gun propellants are correlated with the design characteristics of weapon and ammunition allowing the assessment of the performance and safety features of the whole system.

Experimental testing setup for study of Ti/steel foam/Ti sandwich plate behaviour

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Keywords: ballistic protection; steel foam; sandwich structures.

In order to estimate if a structure, especially the ones used in ballistic protection, will withstand the blast wave, experimental investigations must be carried out. Special test configuration must be design to evaluate the sandwich capacity to absorb the blast impulse. The present paper aims primarily to investigate, by experimental tests, the behavior of a Ti/Steel foam/Ti sandwich plate loaded by a flat head projectile. The study results points towards the idea that the sandwich structures could be successfully tested with proper laboratory equipment.

Physicochemical properties of sorbitol hexanitrate and its solutions in nitroglycerine and diethylene glycol dinitrate

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Keywords: sorbitol hexanitrate; nitroglycerine; diethylene glycol dinitrate.

Physicochemical properties of sorbitol hexanitrate and its solutions in nitroglycerine and diethylene glycol dinitrate have been studied. The temperature and enthalpy of melting, and thermal stability of hexanitroester have been determined, and the solutions of sorbitol tetranitrate in nitroglycerine and diethylene glycol dinitrate have been studied using differential scanning calorimetry. The temperature and enthalpy of melting are 53 °S and 84.6 J/g. An equation has been derived for the constant of sorbitol hexanitrate thermal decomposition. In an isothermal mode (at 60°S), the decomposed hexanitroester amount does not exceed 40,08×10-4 wt % in 60 minutes. The properties of sorbitol hexanitrate–nitroglycerine and sorbitol hexanitrate–diethylene glycol dinitrate two-component solutions have been ascertained. At room temperature (t=20°C) nitroglycerine and diethylene glycol dinitrate dissolve about 21 mol % hexanitroester. These two-component solutions have higher densities and lower volatilities than individual nitroglycerine or diethylene glycol dinitrate. The two-component solutions are completely thermodynamically compatible with polyurethane and divinylnitrile rubbers.

Synthesis and characterization of energetic 1,1,1-trinitropropyl-1-ammonium salts as potential high-energy dense oxidizers

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Keywords: high energy dense oxidizer; polynitro compounds; energetic properties; specific impulse; crystal structure.

The synthesis of 1,1,1-trinitropropyl-1-ammonium salts starting from a nucleophilic MICHAEL ADDITION of nitroform to acrylamide is described. Due to the relatively high oxygen content of the resulting salts their suitability as high-energy dense oxidizers (HEDOs) in energetic formulations were predicted according to their specific impulse and detonation velocity. The parameters were calculated with the EXPLO5 (V6.02) computer code and compared to the common solid rocket propellant ammonium perchlorate (AP). Characterization including multinuclear NMR spectroscopy, vibrational analysis (IR, Raman) as well as elemental analysis and single crystal X-ray diffraction studies were performed. Crystal structures of several salts are presented. The thermal stability was studied using differential scanning calorimetry and the sensitivities against impact, friction and electrostatic discharge were determined. Furthermore, the energies of formation were calculated using GAUSSIAN 09.

Interaction of 1,3-butildiolferrocenylene and 1,1'-bis(1,3-butildiol)ferrocenylene with N-nitrocarbamide

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Keywords: ethyl acetate; N-nitrocarbamide; glacial acetic acid; ferrocene; ferrocenylbutanediol; ferrocenylbutanetetraol.

The interaction of 1,3-butildiolferrocenylene and 1,1'-bis(1,3-bitildiol)ferrocenylene with N-nitrocarbamide. Characteristics and spectral properties of the N-nitrocarbamide derivatives of 1,3-butildiolferrocenylene and 1,1'-bis(1,3-bitildiol)ferrocenylene. Keywords: ethyl acetate; N-nitrocarbamide; glacial acetic acid; ferrocene; ferrocenylbutanediol, ferrocenylbutanetetraol.

Eco-friendly polymeric binders for energetic formulations

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Keywords: binders; polymers; environment; explosives; pyrotechnics.

In the context of worldwide efforts for greener munitions development, the aim of this paper is to present some experimental studies regarding synthesis and characterisation of new generations of greener and safer binders for energetic formulations. These binders can contribute to enhance the safety and reduce the environmental impact of binders in manufacture and recovery/reuse. The first class of binders was designed for recyclable explosive formulations. For this purpose, “smart” polymeric binders were synthesised based on acrylic acid and other acrylic monomers. Their main feature is they are soluble in water at slight alkaline pH allowing facile recovery of explosive fillers without using organic solvents, while maintaining their chemical and physical characteristics. A second class of binders based on polyurea was designed for use in solvent free pyrotechnic compositions. These polymers allow wet or dry pressing of the pyrotechnic compositions without using volatile organic solvents. The rubbery texture of the polyurea minimises the risks associated to the dry pressing of other brittle binders and improves the safety characteristics while maintaining the performance.

Synthesis and evaluation of nitrile oxide as a low-temperature curing agent

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Keywords: nitrile oxides; curing agent; unsaturation binders; cross-linked polymer; rubber.

In this study, two bisnitrile oxides tetramethyl-terephthalobisnitrile oxide(TTNO) and 2,4,6-trimethylisophthtalodinitrile oxide(TINO), two nitrile oxide precursors were prepared and characterized as low-temperature curing agents. 20 g of TTNO were prepared in 4-steps from 1,2,4,5-tetramethylbenzene. A low-temperature curing system based on hydroxyl-terminated polybutadiene (HTPB) and tetramethyl-terephthalobisnitrile oxide(TTNO) was evaluated. TTNO reacts with unsaturated bonds of HTPB to form isoxazoline cross links. Curing of TTNO and HTPB produced good rubber material. Similar, a low-temperature curing system based on liquid polybutadiene (LPB) and tetramethyl-terephthalobisnitrile oxide(TTNO) was evaluated. TTNO reacts with unsaturated bonds of LPB to form isoxazoline cross links. Curing of TTNO and LPB produced good rubber material. The solution of nitrile oxides, preparation of elastomers, microstructure of elastomers, structural characterization, mechanical properties of elastomers were investigated.

Closed bomb burning properties of the single-base gun propellants coated with glycidyl azide polyurethane

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Keywords: glycidyl azide polyurethane; single-base propellant; gun propellant coating; progressive burning.

Abstract: The 7-perforated single base gun propellant grains were coated by spraying method with Glycidyl azide polyurethane, which was adjusted to cure faster. The GAP polyurethane coated single-base propellants were prepared by "pre-mixing, spraying, and curing" method. Differential scanning calorimeter (DSC) was conducted to observe the compatibil-ity of the GAP polyurethane and the single-base propellant. The energetic properties of the propellants were calculated and discussed. The constant-volume burning characteristics were investigated by closed-bomb test. The results show that the coated gun propellant burned steadily up to 250 MPa in closed bomb and a transparent coating layer of GAP polyurethane bonded to single-base gun propellant strongly. The impetus of the propellants coated with GAP polyurethane is higher than that of the single-base propellant coated with inert coating materials. Compared with the single-base propellant without any surface treatment, the relative pressure at split point (Bs) of the single-base propellant coated with 7.0% (by wt.) GAP polyurethane increases from 0.151 to 0.453, and the value of the progression factor (Pr) increases from 0.090 to 0.293, indicating that the potential of burning progressivity with GAP polyurethane coating.

Research on the laser initiation based on STD

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Keywords: laser initiation; charge without initiating explosive; shock initiation.

Laser initiation technology based on STD(Shock To Detonation) has a strong ability of anti-EMI(electromagnetic interference), with which charge without initiating explosive in pyrotechnics can be realized. It satisfies high safety and reliability requirements of pyrotechnic systems for modern battlefields. In this paper, The mechanical behavior of block shocking the secondary charge was studied by numerical simulation method combined with experiments, and the effect of shock-wave convergence was revealed; based on theoretical analysis, a block's velocity model was built and influence characteristics on the block's velocity of the mass of the primary charge, the block's mass and the length of accelerating barrel were researched. It is shown that the initial velocity of the block could be significantly improved by increasing the mass of the primary charge or decreasing the block's mass; RDX makes more contributions to the initial velocity of the block than B/KNO3; the effect on acceleration of increasing the barrel's length is limited and it weakens gradually with the length increasing.

Effects of hard segment contents on cryogenic viscoelasticities of GAP-based polyurethane elastomers

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Keywords: GAPE; TTS; fragility parameter.

Gap-based polyurethane elastomer (GAPE) was synthesized through meltprepolymerization method using 1,4-butanediol (BDO) as chain extender. Dynamic mechanical analysis (DMA) was applied to research the dynamic mechanical properties of GAPE .Then storage modulus, loss modulus and dissipation factor were obtained. Based on the time-temperature superposition theory, master curves with frequency spanning more than ten several orders of magnitude range were obtained. The constants C_{1g} and C_{2g} of WLF equation were calculated. The dynamic mechanical properties parameters, activation energy and fragility parameter of GAPE were obtained. The results show that Tg of GAPE-2 is -18.4°C.What's more the low-temperature fragility parameter and activation energy of GAPE-2 were lower, respectively, 55.6 and 271.0 KJ•molsup>-1</sup>.

Energetic materials with promising properties: synthesis and characterization of polynitro compounds

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Keywords: energetic materials; polynitro compounds; esteryl-bridged; crystal structure.

Abstract: Four energetic polynitro derivatives were designed, synthesized, and fully characterized. The structures of the resulting compounds 2,2,2-trinitroethyl 2,4,6-trinitrobenzoate(5), bis(2,2,2-trinitroethyl) 4,6-dinitroisophthalate(6), bis(2,2,2-trinitroethyl) 2,5-dinitroterephthalate(7) and bis(2,2,2-trinitroethyl) 2,4,6-trinitroisophthalate (8) were further confirmed by X-ray diffraction studies. Physicochemical and energetic properties including density, thermal stability, and sensitivity were investigated, and energetic properties (e.g., detonation velocities and detonation pressures) were calculated using EXPLO5 code. Most of the polynitro esters decompose at temperatures over 180 °C (except for 6 : 171.6 °C), exhibit good thermal stability. Furthermore, the performance calculations gave detonation pressures and velocities for the ester derivatives in a range of 30.4-32.9 GPa and 8267-8559 m s-1, respectively. The esteryl-bridged compounds possess acceptable impact sensitivities (14-22 J), friction sensitivities (240–360 N), and electrostatic sensitivities (0.20-0.32 J). Thus, these compounds could be candidates as promising energetic materials. Keywords: energetic materials; polynitro; esteryl-bridged; crystal structure

Hybrid ballistic gels - Dynamic impact evaluation

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Keywords: gelatin; ballistic tests; v50; Gamo.

After validating the physicochemical and mechanical properties requirements of the hybrid ballistic gels, the product must be validated in terms of dynamic impact versus standard ballistic gelatin. Testing and evaluation against dynamic impact of the ex-perimental model refers to the stab and shooting behavior of ballistic gelatin against various types of cartridges.

Investigation on the stability of multisubstituted arylpentazoles and the influence on the generation of pentazolate anion

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Keywords: pentazolate anion; arylpentazole.

A series of mono-, di- and tri-substituted arylpentazoles were synthesized from various substituted anilines. The effects of the number and position of the substituents on the arylpentazoles stability were investigated at different temperatures. Electrospray ionization tandem mass spectrometry was used to infer the decomposition pathway of arylpentazoles. The relationship between the arylpentazole stability and the relative intensity of the generated pentazolate anion was studied.

The influence of elevated temperature of accelerated ageing according to STANAG 4620 method on molecular weight distribution of nitrocellulose

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Keywords: size exclusion chromatography; molecular weight distribution; nitrocellulose; accelerated ageing; STANAG 4620.

Nitrocellulose powders are commonly used as high energetic materials in combat means as a propelling charge. Unfortunately, during long-term storage degradation of nitrocellulose occurs. This process leads to decrease of average molecular weights and is dependant not only on time but also on storage temperature. Nitrocellulose exhibits differing physical and chemical properties together with molecular weight distribution changes. To determine whether nitrocellulose powders can be exploited safely after prolonged time of storage researchers create methods of accelerated ageing which simulate real-time behaviour of propellants. Accelerated ageing of chosen propellants was conducted according to procedure proposed in STANAG 4620. In this work there are presented the investigation results of influence of elevated temperature of accelerated ageing according to STANAG 4620 method on molecular weight distribution of nitrocellulose. To determine average molecular weight distribution the size exclusion chromatography method (SEC) with photodiode detector (UV) was used.

“Hot plate” laser ignition of the condensed energetic material

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Keywords: laser ignition; energetic materials; PETN; copper (II) oxide; heat transfer simulations.

Laser initiation of polycrystalline PETN tablet coating with copper (II) oxide was studied. An ytterbium fiber laser with 1070 nm wavelength, 20 ms pulse duration and 3.6 kW/cm^2 power density was used. Probability of sample explosion and reaction zone formation as a function of energy density was registered. Four series of samples with CuO thickness 9-18μm was used in experiment. The effectiveness of the initiation of the explosion decreases with the increase in the thickness of the absorbing layer. An analytical model describing the initiation of the exothermic decomposition reaction in the surface layer of the sample was developed. Critical energy density necessary for ignition as a function of CuO layer thickness was calculated. Calculated values good correlate with experimental one for two minimal thicknesses. Discrepancy between experiment and calculated critical ignition energies for thicker coatings was apparently explained by CuO layer destruction until ignition of the PETN.

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