Abstracts of the 12th Seminar on

New Trends in Research of Energetic Materials

Pardubice, April 1–3, 2009

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

supported by

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

Abstracts of the 12th Seminar on

New Trends in Research of Energetic Materials

Held at the University of Pardubice

Pardubice, Czech Republic
April 1–3, 2009

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

This publication has not been submitted to language corrections and contributions have not been reviewed.

This is freely available proceedings of abstracts. The full proceedings (978-80-7395-156-6) can be ordered or gained by exchange of similar pulications at the address:

Institute of Energetic Materials
University of Pardubice
532 10 Pardubice
Czech Republic

NTREM '09

Abstracts of Seminar on New Trends in Research of Energetic Materials

Jiri Pachman, Jakub Selesovsky, Robert Matyas (editors).
Conference and proceedings number: 12.
Published by University of Pardubice.
Czech Republic, April, 2009.
128 pages.
Checked by editor, typeset and completed by Vít Zýka (www.typokvitek.com).

Chairman of the Seminar:

Prof. Svatopluk Zeman, D.Sc.	*IEM, FCT, University of Pardubice, CR*

Scientific Committee:

Chairman

Dr. Adam Cumming	*DSTL, Sevenoaks, UK*

Members

Prof. How-Ghee Ang	*Nanyang Technological University, Singapore*
Prof. Alexandr Astachov	*Siberian State Technological University, Russia*
Dr. Anthony J. Bellamy	*Cranfield University, UK*
Dr. Stanislaw Cudzilo	*Military University of Technology, Warsaw, Poland*
Dr. Ruth Doherty	*Department of Homeland Security, Washington, USA*
Prof. Zdenek Friedl	*Brno University of Technology, CR*
Prof. Manfred Held	*EADS/TDW, Schrobenhausen, Germany*
Prof. Thomas Klapoetke	*Ludwig Maximilians Universitat, Munchen, Germany*
Prof. Michel Lefebvre	*Royal Military Academy, Belgium*
Dr. Carl-Otto Leiber	*Rheinbach, Germany*
Prof. Frantisek Ludvik	*University of Defence, Brno, CR*
Prof. Andrzej Maranda	*Military University of Technology, Warsaw, Poland*
Prof. Hans J. Pasman	*Delft University of Technology, The Netherlands*
Prof. Tatiyana S. Pivina	*Zelinskii Institute of Organic Chemistry, Moscow, Russia*
Prof. Peter Politzer	*University of New Orleans, USA*
Dr. Scott A. Shackelford	*AFRL/PRSP, Edwards AFB, USA*
Prof. Yuan-jie Shu	*Institute of Chemical Materials, CAEP, Sichuan, China*
Prof. Valerii P. Sinditskii	*Mendeleev University of Chemical Technology, Russia*
Dr. Muhamed Suceska	*Brodarski Institute, Zagreb, Croatia*
Assoc. Prof. Pavel Vavra	*IEM, FCT, University of Pardubice, CR*
Dr. Woodward Waesche	*SAIC, Gaineswille, USA*

Organizing Committee:

Chairman

Dr. Jiri Pachman	*IEM, FCT, University of Pardubice, CR*

Members

Assoc. Prof. Ladislav Lehky	*Explosia, Pardubice, CR*
Dr. Jan Jakubko	*Indet Safety Systems, Vsetin, CR*
Dr. Marcela Jungova	*IEM, FCT, University of Pardubice, CR*
Dr. Pavel Valenta	*Austin Detonator, Vsetin, CR*
Dr. Iva Ulbrichova	*Dean office, FCT, University of Pardubice, CR*

Seminar is supported by:

U.S. Army International Technology Center – Atlantic, London
Office of Naval Research Global, Middlesex
Austin Detonator, Vsetin
Indet Safety Systems, Vsetin, a member of Nippon Kayaku group
Explosia, Pardubice
Faculty of Chemical Technology, University of Pardubice, Pardubice
STV Group, Prague
OZM Research, Bliznovice
BORGATA, Prague

Contents

Part 1

Part 2

Posters

Preface

This is the twelfth seminar *New Trends in Research of Energetic Materials (NTREM)* and the eleventh in the series of seminars organised by the Institute of Energetic Materials (IEM) of the University of Pardubice. The original stimulus for starting these meetings was an attempt to teach young researchers to present their results in front of scientific audience. Over the years it evolved into a meeting of people involved in scientific and research activities in the field of energetic materials with emphasis on academic research. The international seminar NTREM represents one of the most significant activities of IEM. It gives our student excellent opportunity to enhance their education by direct participation in all activities related to the meeting.

Realization of our seminars would never be possible without the generous support of many institutions. The twelfth NTREM seminar has been financially supported by:

- United States Army International Technology Center-Atlantic, London U.K. (conference grant)
- U.S. Office of Naval Research Global, Middlesex, U.K. (conference grant)
- Austin Detonator, Vsetín, Czech Republic
- Explosia, Pardubice, Czech Republic
- Indet Safety Systems, Vsetín, Czech Republic (member of Nippon Kayaku group)
- STV Group, Rataje u Kroměříže, Czech Republic
- Faculty of Chemical Technology, Pardubice, Czech Republic
- OZM Reasearch, Hrochův Týnec, Czech Republic
- BORGATA, Prague, Czech Republic

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

The contributions presented at NTREM have been abstracted by Chemical Abstracts since the third seminar in 2000. The lasting interest in the topic of the seminar can be demonstrated by the numbers in the following table:

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	26	100	~200

The past meetings have proved to be an excellent opportunity not just for the exchange of scientific and technological information but also for establishing personal contacts amongst many scientists from variety of different countries. The personal contacts gained during past seminars have laid essential base for opening cooperation of the Institute of Energetic Materials with many institutions including Military University of Technology in Warsaw, Cavendish Laboratory of the University of Cambridge, Institute of Industrial Organic Chemistry in Warsaw, Middle East Technical University in Ankara, Institute of Chemical Materials of the China Academy of Engineering Physics in Mianyang, Nanjing University of Science and Technology in Nanjing, Nanjang Technological University in Singapore and Ludwig-Maximilians-University in Munich.

Well, what should I add on the occasion of this 12th NTREM seminar? First of all, I would like to express the wish: May its proceedings be successful and may it bring inspiration and pieces of knowledge for use in further scientific research activities in the area of energetic materials, may it enable establishing new contacts and deepen the existing ones particularly between the young participants of this meeting. I wish for the participants to find a pleasant welcoming atmosphere throughout the seminar. Finally, I wish to thank the members of the Scientific Committee, the authors of all the submitted papers and, last but not least, you, the participants in this seminar, for its success and its influence on the continued success and growth of all future meetings at our University.

Pardubice, February 27, 2009

Svatopluk Zeman

Lessons Learned through Research Collaboration - A View over 20 Years

Adam S. Cumming

Dstl

ascumming@compuserve.com

Keywords: research collaboration; energetic materials.

Over the last twenty years Europe has become increasingly involved in government led research collaboration in Energetic Materials. Starting from simple bilateral activities these have developed to multilateral programmes an included support from secretariats and forums aimed at supporting and coordinating opportunities. The success rate has been high, but not uniform, and the reasons for this will be discussed, together with examples of the output of the various programmes. The role of NATO, WEAG and EDA will also be described and the author's view of key success factors will be given. Links beyond Europe will also be briefly discussed.

Blast Load Diagnostic

Manfred Held

tdw

manfred.held@mbda-systems.de

Keywords: blast load diagnostic.

Damage of blast waves is generally caused by the transferred impulse. Therefore this value has to be measured, what can be achieved with nearly simple and not expensive methods. Presented are examples of momentum gauges as cubes, or plates and pistons.

Training film to laboratory practical work of students on theory of burning and explosion

Svetlana Kazakova, Georgii Kozak, Anna Kuznetsova

Mendelejev University of Chemical Technology

Keywords: laboratory practical work; training film; burning; heat explosion; impact.

Theory of burning and explosion is the component of curriculums at some specialists grounding in higher school. Teaching method based on lectures and seminars we usually supplement with laboratory practical work. Some laboratory works students carry out with assistance of teachers, another ones that relate with higher risk are shown to students in demonstrational variant. During the first introductory lecture students familiarize with safety measures at working with dangerous materials and then a teacher demonstrate some experiments. Our contribution is the video film with these experiments. Burning of some secondary high explosives (Tetryl, HMX, RDX etc.) ,pyroxylin, black powder, ballistite in air and in water are demonstrated in video film. Firing and explosion of small quantity of lead azide on glass plate clearly show that this substance detonates and perforates glass plate. Next experiments in the film demonstrate heat explosion of Tetryl and explosion of small quantity of PETN at impact with a hummer. The frames of film with descriptions of experiments are included into article.

Environmental aspects in the research of energetic materials

Thomas M. Klapötke

Ludwig-Maximilian University of Munich

tmk@cup.uni-muenchen.de

Keywords: energetic materials; environment.

In this contribution various aspects of environmental concerns relating to energetic materials will be discussed. Topics included range from RDX replacements, over lead-free primary explosives and high-nitrogen propellant charges to environmentally compatible colorants in signal flares.

Practical Safety Concepts: Structured thinking conditional for optimum EM work

Hans J. Pasman

Mary Kay O'Connor Process Safety
Center, Texas A&M University, TX

hjpasman@gmail.com

Keywords: safety at work; risk analysis; layers of protection; safety attitude.

In all activities of life there is a certain risk one will hurt him- or herself while in a mishap also others can be affected. In EM work this will not be different, but because of the potential and reputation of EM special care shall be taken. The paper will show how difficult it is to get a complete picture on the forehand what can go wrong; it will reveal how scenarios can be generated best, how risk shall be estimated by simple means and what we can do to reduce probability and severity. Briefly will be explained the distinction between personal, process and laboratory safety. Finally the importance of safety culture will be underlined.

Study of using thermochemical calculations for determination of TNT equivalent of CHNO explosives

Zoran Bajić, Jovica Bogdanov

Military academy

zbajic@sezampro.rs

Keywords: BKW-RR; BKW-RDX; TNT equivalent; CHNO explosives.

This paper analyses an approach of using thermochemical calculations of detonation parameters of standard CHNO explosives for determination of TNT equivalent. Thermochemical calculations are based on BKW-RR and BKW-RDX equations of state depending on type of explosive.

A Simple Antisolvent Phase Separation Process for Purification of RDX

Veera Boddu, Krishnaiah Abburi, Reddy Damavarapu

U.S. Army Engineer Research and Development Center, CERL, Illinois
U.S. Army - Armament Research, Development
and Engineering Center, New Jersey

veera.boddu@usace.army.mil, abburikrishnaiah@gmail.com

Keywords: insenstive RDX; antisolvent process.

The sensitivity of explosive compounds depends on their purity. Reduced Sensitivity (RS) or Insensitive Munitions (IM) are desired for reasons of safe load, assemble, and pack (LAP) operations and to meet the safe handling requirements of the end user, the soldier. This presentation describes a separation process for two of the most widely used explosive compounds, RDX (1,3,5-Trinitro-1,3, 5-triazacyclohexane) and HMX (1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane). The crude product formed during the manufacturing process is filtered and recrystallized to form RDX. The RDX produced by the industrial process usually contains about 8-12% HMX. The sensitivity of the final explosive depends on the relative composition of RDX and HMX. The sensitivity of the crude RDX increases with increase in composition of HMX. We have developed a simple separation process to obtain >99% pure RDX from crude RDX, consisting of RDX ($\approx$ 90%) and HMX ($\approx$ 10%). The process uses a solvent that dissolves crude RDX and uses another solvent that preferentially precipitates RDX. The air dried precipitate of the RDX was analyzed for its purity using chromatography. Other functional group analysis was conducted using the Fourier Transform Infrared (FTIR), and Proton Nuclear Magnetic Resonance (1H NMR) spectral methods. To study the crystalline structure of the RDX, X-ray diffraction (XRD) patterns were also obtained. Analysis of the separation process and spectral information shows that relatively pure RDX can be obtained from the crude RDX following the simple phase separation process. Details of the separation process including effect of temperature and ratio of solvents will be presented.

Ageing Behaviour of HTPB based Rocket Propellant Formulations

Sara Cerri, Manfred A. Bohn, Klaus Menke, Luciano Galfetti

Fraunhofer-Institut fuer Chemische Technologie (ICT)
SPLab Dipartimento di Ing.
Aerospaziale, Politecnico di Milano

sara.cerri@ict.fraunhofer.de, manfred.bohn@ict.fraunhofer.de

Keywords: ageing of composite RP; influence of nano aluminium; change in mechanical properties.

The ageing of mechanical and ballistic properties of aged HTPB-based solid propellant have been studied already. But only a few works have investigated the impact of nano-particles on the mechanical properties and on the ageing behaviour. Because of inserting nano-Al important increases in the ballistic performances as burning rates and gravimetric specific impulse can be obtained, the ageing of such material is an essential aspect of performance evaluation. Consequently, an investigation of the ageing behaviour on the kinetic mechanisms, multiple aspect of sensitivity, and on the mechanical properties was undertaken. During natural ageing the material undergoes a series of slow chemical-physical degradation reactions (plasticizer migration, antioxidant consumption, oxidative ageing, additional cross-linking, chain scissions ...). By using accelerated ageing conditions it is possible to simulate the material behaviour at different time-temperature conditions especially focused on in-service conditions.

Several HTPB/AP/Al propellant formulations have been manufactured freshly and were investigated in unaged and aged conditions. All the formulations contain 16 mass-% of binder, consisting of HTPB-IPDI, plasticizer and antioxidant. Two families of materials having 6 mass-% and 12 mass-% of aluminium content were compared. In order not to get too high values of casting viscosity the nano-aluminium content was limited to 6 mass-%. The ballistic performances of the propellant formulations were calculated using the ICT-Thermodynamic code. EDX analyses of the unaged materials and SEM analyses of the unaged and aged materials were made using the scanning electron microscope of type Supra 55 VP from Carl Zeiss SMT AG, Germany. Uniaxial tensile tests were conducted at room temperature using three different strain rates (0.00167, 0.0167, 0.167 s-1). DMA analysis in torsion mode and DSC measurements was performed with the purpose to investigate changes in the glass transition temperature of the materials and the presence or absence of secondary phenomena. Obtained results indicate differences in ageing behaviour of formulations containing nano-Al.

Shock waves generated by the firing of small caliber weapon systems

Marius Valeriu Cirmaci, Doru Adrian Goga

Military Technical Academy

mariusvaleriu@yahoo.com

Keywords: shock waves; small arms; safety; suitability.

The goal of this article is to present experimental procedures and their results, regarding shock waves generated when firing small caliber ammunition, like 9x19 Parabellum cartridge. For a new armament system, the safety and suitability for service requirements impose a good knowledge of interaction between the gunner and the armament system. One of the consequences of the fire shot is strictly connected with the expansion of hot and high pressure combustion gases, liberated at the muzzle. The amplitude of the shock wave can disturb the gunner or the neighbours, and can affect other devices mounted on the gun. The experimental results for shock wave generated when firing small caliber ammunition reveals an analogy with the shock wave generated by detonation of an explosive material. The pressure measurements are related to a polar coordinate system linked to the firearm. The interaction between the gunner and the shock wave is evaluated by measuring acceleration of the body and the sound characteristics.

Preparation and characterization of resorcinol-formaldehyde gels impregnated with ammonium chlorate(VII) and nitrate(V)

Stanislaw Cudzilo, Waldemar Trzcinski, Wojciech Kicinski

Military University of Technology

scudzilo@wat.edu.pl

Keywords: energetic nano-composites; sol-gel; freeze-drying; sensitivity; mechanical stimuli.

Abstract: Energetic nano-composites were prepared via polycondensation of resorcinol and formaldehyde in concentrated solutions of ammonium chlorate(VII) and nitrate(V) in water. The obtained gels were rapidly frozen and next freeze-dried. The microstructure of the resulting composites was studied using scanning electron microscopy as well as some of their explosive properties were experimentally determined, i.e. the sensitiveness to mechanical and thermal stimuli, sensitivity to detonation. Detonation parameters of the explosives were calculated using Cheetah code.

Novel melt cast energetic ingredients

Reddy Damavarapu

ARDEC;Picatinny, NJ

reddy.damavarapu@us.army.mil

Keywords: melt-cast; energetic.

In modern ordnance there is a strong requirement for explosives having good thermal stability, impact insensitivity and energetic performance. However, these requirements are somewhat mutually exclusive. The explosives having good thermal stability and impact insensitivity usually exhibit poor explosive performances and vice versa. As a part of a program to develop more powerful explosives and propellants, we have designed a new class of explosives based on substituted nitroimidazoles. Synthetic efforts towards the preparation of these polynitroimidazoles will be presented.

A comparative study on cyclic acetone peroxides

Viacheslav Egorshev, Valery Sinditskii, Sergei Smirnov, Evgeny Glinkovsky, Viacheslav Kuzmin

Mendelejev University of Chemical Technology

Keywords: acetone peroxides; DATP; TATP; thermal decomposition; combustion; vapor pressure; burning rate.

Two potentially initiating explosive compounds, diacetonediperoxide (DADP) and triacetonetriperoxide (TATP), have been studied in respect to thermal decomposition, burning behavior, impact sensitivity, and initiating ability. For the first time for DADP, vapor pressure and burning rate have been measured. The kinetic parameters of decomposition of the peroxides in the gas phase were obtained in the temperature interval of 150-200 C. The decomposition reactions of DADP and TATP were determined to follow the first order to high degree of decay with the close activation energies of 39.9 and 42.5 kcal/mole. The decomposition rate constant of DADP was found to be approximately four times less than that of TATP. On the whole, the thermal stability of the studied peroxides was higher than the thermal stability of nitroesters and approached to that of alkyl azides. The linear burning rate of DADP was measured to be approximately five times less than that of TATP. Temperature profiles in combustion waves were measured at subatmospheric pressures with thin thermocouples. The leading reaction on combustion of both peroxides was proposed to occur in the gas phase. The kinetic parameters of this reaction derived from combustion data corresponded to the kinetic parameters of low-temperature thermal decomposition if extrapolated to the high-temperature zone. Sensitivity to drop-weight impact was measured comparatively for the peroxides. DADP showed notably less sensitiveness than TATP. No deflagration-to-detonation transition was observed when RDX was attempted to explode by 0.5 gram of DADP in the shell of standard detonator. Comparing explosive properties of the studied peroxides, DADP can be considered as a less dangerous in handling explosive than TATP.

The Validation of the Explosive Fumes Dynamics in Rooms

Hans-Jürgen Fahl

Bundeswehr Technical Center
for Weapons and Ammunition

hansjuergenfahl@bwb.org

Keywords: simulation; AUTODYN; SIBEX; explosives; fume; dynamic; validation.

Last year the discovery of the explosive fumes dynamics in rooms was published. The fumes dynamics of TNT had been observed up to now only by numerical simulations with the software AUTODYN®6.1z. To validate the fumes dynamics within the first 10 ms after the detonation, a test room was equipped in the urban module in Meppen with different measuring sensors. For the first time high speed heat flow sensors were used in the test room parallel to numerous pressure and temperature sensors resulting from cooperation with the German-French Research Institute Saint-Louis (ISL). The position of the hot fumes cloud could be determined exactly by the installation of the measuring sensors close to each other and by the triggering of the measuring signals at the same time. Optical tests of validation took place in addition also in the Fraunhofer Ernst-Mach-Institute (EMI) in the laboratory scale (1:10). The measurements and optical pictures confirm in principle the existence of the fumes dynamics of TNT in rooms. There for, the simulation results of the software AUTODYN® 6.1z are also validated in principle. Then with other planned basic experiments in the urban module should be determined the beginning of the after burn effect with aluminium-containing SIBEX explosives (Shock Insensitive Blast Enhanced EXplosives) and the influence by turbulence/mixture-effects in rooms with different atmospheres (air and argon).

Numerical Simulation of Non-ideal Detonation of Condensed Explosives

Xiaomian Hu, Junxia Cheng, Hao Pan, Kun Yang

Institute of Applied Physics and
Computational Mathematics

hu_xiaomian@iapcm.ac.cn

Keywords: non-ideal detonation; detonation shock dynamics; equation of state.

A new reaction model is bulit up by thinking of the excitation process and slow reaction in the detonation process of insensitive high explosives (IHE). This reaction model can be used in coarse mesh as compared with other reaction model. In the mesh of 50 cells per centimeter, the calculated results of the free surface velocity of copper flyer driven by JOB-9003 and JB-9014 are according with the experiment data. We also apply this model to calculate the process of IHE driving LiF. In the mesh of 50 cells pre centimeter, the calculated result of the interface between LiF and IHE is according with the experiment data. When the mesh size is smaller, the error between them is smaller. It indicates that this new model can describe the process of driven flyers by IHE in coarse mesh, and it can be widely used in practical works. Employing the Davis equation of state, the expansion of metallic tubes induced by two head-on colliding detonation waves inside has been studied. The parameters of Davis EOS of JOB9003 are calibrated in the 2-D hydrokinetics program. Used the program to simulate the experiment of the expansion of metallic tubes induced by two head-on colliding detonation waves inside, the results are according with the experimental results. We also compare the results with the results calculated by JWL EOS. It indicates that Davis EOS can describe this experiment more accurately than JWL EOS. Detonation shock dynamics describes the diameter effect of condensed explosives with the relationship of detonation speed and curvature, and level set method solves the equations of detonation speed and curvature on arbitrary quadrilaterals.

Study on Mechanical of Properties of Plasticity Explosive and Influenced by Temperature and Time

Junxia Cheng

Institute of Applied Physics and
Computational Mathematics

cheng_junxia@iapcm.ac.cn

Keywords: explosives; plasticity explosive; time-temperature superposition (TTS); mechanical properties.

The present paper aims at studying the mechanical properties of the plasticity explosives through analyzing the experimental data of such explosives by using the Time-Temperature Superposition (TTS) principle. Further studies reveal the influence of time and temperature on the properties of different plasticity explosives based on the application of TTS principle.

Ageing of a Spherical and a Flattened Propellant

Laurence Jeunieau, Michel H. Lefebvre, Pierre Guillaume

Royal Military Academy
PB Clermont

laurence.jeunieau@rma.ac.be, michel.lefebvre@rma.ac.be

Keywords: propellants; ageing; influence of propellant geometry.

Ball powders are used in many small-bore applications. They are easy to manufacture and can be designed for different ammunition types by modification of their surface. This surface modification usually consists of an impregnation by a deterrent which is only present along the surface up to a certain depth. This contributes to maintain a nearly constant pressure generation during most of the combustion, because the burning rate increases with time, compensating for the decreasing burning surface. In this work, the ageing characteristics of a flattened and a spherical deterred propellant have been investigated. The flattened propellant has been manufactured by flattening the spherical propellant. Consequently both propellants have exactly the same chemical composition. These propellants have been aged at different temperatures and the aged propellants have been characterized by infrared-microscopy, closed vessel tests and differential scanning calorimetry. The infra-red microscopy has permitted to observe the deterrent migration during ageing and to quantify its diffusion properties. The deterrent migration is more pronounced for the flattened propellant than for the spherical propellant. Consistently, the closed vessel tests show an increase of the combustion rate at the low value of pressure due to the deterrent migration. An increase of the combustion rate is also observed for the high pressure value, this one could be explained by a decrease of the nitrocellulose molecular weight. The differential scanning calorimetry shows a general decrease of the decomposition temperature with ageing. This decrease is somehow greater for the flattened propellant than for the spherical one.

Crystallization of 1,1-diamino-2,2-dinitroethylene by drowning-out

Jae-Kyeong Kim, Jin-Hwan An, Jun-Woo Kim, Hyoun-Soo Kim, Kee-Kahb Koo

Sogang University
Agency for Defense Development

tetrapodfish@empal.com

Keywords: DADNE; crystallization; drowning-out.

Current studies on 1,1-diamino-2,2-dinitroethylene (DADNE) show that DADNE has signifi-cantly low friction and impact sensitivity than 1,3,5-trinitroperhydro-1,3,5-triazine (RDX), but has similar energetic performance. The insensitive characteristics give powerful applications for the LOVA (low vulnerability ammunition) system. Such munitions need to control size dis-tribution and morphology of DADNE crystals which are important factors on ballistic behav-iour in military propulsion system. Crystallization process therefore is essential to control those particulate characteristics. In the present work, a drowning-out crystallization was employed and various pairs of solvent/anti-solvent were tested with saturation temperatures, flow rates of solution and mixing ratio as experimental variables. Polyhedron-shaped crystals of DADNE with size of 5 – 30 micrometer were obtained and they were characterized by IR, SEM, and DSC.

Azole-Based Energetic Materials: Advances in Nitrogen-rich Chemistry

Thomas M. Klapötke, Carles Miró Sabaté

Ludwig-Maximilian University of Munich

Keywords: azoles; synthesis; energetic compounds; performance; safety testing.

Triazole and, in particular, tetrazole-based energetic materials have been the focus of our investigations during the last couple of years. This paper intends to present straightforward syntheses, characterization and initial safety testing results of new azole-based materials with particular attention to selected highlights. At first instance, 5-amino-1H-tetrazole (5-AT) is introduced as a valuable and easily accessible starting material for the synthesis of highly endothermic 5,5'-azotetrazolate salts. Methylation of 5-AT gives a mixture of 1-methyl- (1MAT) and 2-methyl- (2MAT) -5-amino-1H-tetrazoles, which are, in turn, valuable building blocks for the synthesis of neutral 5,5´-azotetrazoles as well as of polymethylated tetrazolium salts with different substitution patterns. The formal replacement of a proton by a silver cation in the latter tetrazolium salts renders a fully new and uninvestigated family of energetic silver salts with high sensitivities. 5-AT can also be derivatized to form the more energetic 5-nitro-2H-tetrazole (5-NT) and the potential of its alkali metal salts as environmentally friendly replacements for service lead(II) azide was studied. Reduction of the azo bridge in 5,5'-azotetrazolate salts leads to the formation of another highly interesting 5-substituted tetrazole, namely, 5-hydrazinebistetrazole, which is unexpectedly stable and energetic. Lastly, the state of knowledge is introduced and the potential of 5-NT to form bridged bistetrazoles is presented, which opens the possibility for new pathways for the synthesis of energetic materials.

Fluorescence analysis technique of explosive detection

Yong Liu, Yuan-jie Shu, Xue-yong Liu, Ying Xiong, Fa-chun Zhong, Yi Sun

China Academy of Engineering Physics

liuychem@gmail.com

Keywords: explosive detection; fluorescence analysis; conjugated polymer.

There are many kinds of explosives, and their detection methods are different vary. Nitroaromatic compounds is one of the composition of the explosives used in common. The fluorescence will be quenched when they touch the fluorescent conjugated polymers. The general methods for explosives detection have been summarized in this paper, in addition the application of novel fluorescence analysis technique in explosives detection has been introduced. The development of fluorescence analysis used in the area of determining explosives has been prospected.

Phenomenon of the Waves of Negative Erosion and Ballistic Efficiency of the High-Loading-Density Solid Propulsion System

Alexander Lukin

Southern Branch of the Russian State Hydro-Meteorological
University of Saint-Petersburg

alexander_lukin@yahoo.com

Keywords: combustion instability; ignition transient; energetic performances; micro-torch structures.

Combustion instability, widely recognized as the most challenging propulsion issue of our day requires continuation of researches. Research of the processes of non-stationary burning and anomalies of burning of the energetic materials (EM) opens possibilities for improvement of theories of burning of the EM. In the paper considered the problem of control of the unstable physical fields in the stagnation zones of the high-loading-density solid propulsion system (SPS) during the ignition-transient period of operation. Within earlier suggested concept of the phenomenon of "negative erosion" the phenomenon of excitation of waves of "negative erosion" is analysed. This is one of typical anomalies of burning. Propagation of the pressure waves in the non-flowing end-face clearances and other stagnation zones will induce waves of "negative erosion" that leads to the mode of pulsating ignition of the charge. The phenomenon of waves of "negative erosion“ will reduce the solid propellant energetic performances. However, the problem of optimum mode of ignition of the stagnation zones is not solved till now. Excitation of the periodic toroidal vortex micro-structures over the burning surface that determine development of the phenomenon of ”negative erosion“ was not taken into account earlier. At the same time, excitation of the thermo-electric convection in the liquid-viscous layer and formation of the micro-torch periodic structures on the EM burning surface is a primary factor for realization of the phenomenon of "negative erosion". During ignition of the charges with stagnation zones arise the reverse flows from the surface of the charge which essentially aggravate the efficiency of the ignition system and leads to increase of the ignition-transient period and to increase of necessary mass of the ignition charge. Use of traditional techniques of ignition does not give possibility to increase the ballistic efficiency of the SPS. The appropriate technologies and ignition system designs for improvement the ballistic efficiency of the SPS are developed. Also, new possibilities of practical use of processes of solid-flame burning of the nano-dimensional multilayered foils and foamed propellants for increase in ballistic efficiency of the SPS are considered.

Mechanical Activation of Al/MoO_3 Thermite as a Component of Energetic Condensed Systems to Increase its Efficiency

Dmitry Meerov, Dmitry Ivanov, Konstantin Monogarov, Nikita Muravyev, Alla Pivkina, Yurii Frolov, Igor Fomenkov

Semenov Institute of Chemical Physics, Russian Academy of Science
Zelinsky Institute of Organic Chemistry
Russian Academy of Science

mmeerov@mail.ru

Keywords: thermites; burning rates; nano-MoO_3.

In the present work a stoichiometric energetic compositions Al+MoO3 prepared by dry mixing and by reactive milling of micro scale particles were investigated. Morphology, particle size and surface structure of produced powders were examined using scanning electron microscopy, atomic-force microscopy, laser diffractometry and BET analysis. DSC/TG data were processed to obtain kinetic parameters describing the reaction between Al and MoO3. The combustion rate of Al+MoO3 thermite mixture increases with pressure, reaching a maximum at 10 atm, and then decreases with further pressure increase. The rise of combustion rate at the low range of pressure is associated with the rise in the extent of the vapour phase penetrating the pores of the pressed sample as the ambient pressure increases. However, at a higher pressure the gas formation is suppressed, and the melt formed in the combustion process can selectively wet the pores resulting in inhibition of reaction. Burning rates of mechanical activated system Al+MoO3 is two times higher then not-activated system at ambient pressure 10 atm and 8 times higher at 40 atm. In additional experiments, nano-scale MoO3 powder was prepared by evaporation with a subsequent condensation onto cooled plate in an inert-gas flow. Scanning electron microscopy showed that nano-MoO3 particles are absolutely spherical with mean diameter 100 nm, and atomic-force microscopy reveals smaller particles with mean diameter 10-30 nm. DSC/TG data showed that the nano-MoO3 starts to sublime earlier than micro MoO3. The use of nano-sized components could considerably increase the burning rates of energetic condensed systems, because of its large specific surface, lower temperature of sublimation, and high reaction ability.

An analysis of test methods on physicochemical properties of solid rocket propellants on the basis of Polish standards

Maciej Miszczak, Jacek Borkowski, Henryk Terenowski

Military Institute of Armament Technology

m.miszczak@chello.pl

Keywords: rocket propellants; physicochemical properties; test methods; standards.

An analysis and discussion on determination and assessment of physicochemical properties of homogeneous and heterogeneous (composite) solid rocket propellants on the basis of Polish currently valid standardization documents such as Defense Standards and Polish Standards respectively for obligatory usage in Polish Military Forces and for non indispensable application, are presented. Defense Standards deal mainly with mechanical characterization of solid rocket propellants including measurements of tensile, compressive, impact strength, Young's and shear moduli, and glass transition temperature. One of Defense Standards describes two test methods on chemical, important characteristic of homogeneous (double-base) solid rocket propellants i.e. their chemical stability measured by evolution of nitro-oxides and depletion of initial stabilizer content during accelerated ageing at relatively high temperature. Polish Standards describe tests concerning thermal, chemical and structure characterization of solid rocket propellants including int. al. determination of their thermal stability, burning rate measurement by small rocket motors, sensitiveness to impact and friction and structure integrity of solid rocket propellants grains through detection of their defects like voids, fissures and debonding between propellant load and its coating. On the basis of analysis and discussion presented in this paper it appears necessity for further development in Poland research and analytical studies including works in standardization area to achieve progress in specification and selection of test methods and assessment criteria for solid rocket propellants esp. taking into consideration implementation of NATO standards into Polish Military Forces. First of all should be implemented and/or developed solid rocket propellants test methods based on DSC, TGA for their thermal characterization and chemical compatibility properties determination. In the range of mechanical/strength parameters of solid rocket propellants, DMA and stress relaxation and/or other rheological tests methods should be developed and implemented as well.

Combustion of energetic systems based on HMX and aluminum: Influence of particle size and mixing technology

Nikita Muravyev, Yurii Frolov, Alla Pivkina, Konstantin Monogarov, Dmitry Ivanov, Dmitry Meerov, Igor Fomenkov

Semenov Institute of Chemical Physics Russian Academy of Science
Zelinsky Institute of Organic Chemistry
Russian Academy of Science

muravyev-nikita@ya.ru

Keywords: energetic systems; burning rate; HMX; aluminium.

In this work the complex experimental investigation of the microstructure and burning parameters of HMX-monopropellant and 25%Al/75%HMX energetic systems was carried on with the particle size variation. Components, their mixtures, pressed samples, and the combustion products (agglomerates) collected from a burning surface by QPCB (quench particle collection bomb) technique were investigated. Two types of HMX particles: micro-sized (mHMX) and ultra fine (uHMX), synthesized by a cryochemical technique were studied. Aluminium powders were also micro- and ultra-sized (ALEXTM). Morphology and particle size were examined by atomic-force microscopy (AFM), scanning electron microscopy (SEM) and BET-analysis. SEM analysis reveals that particles of micro-sized aluminium are spherical to have an average volume diameter 3.3 μm. AFM analysis shows the ALEXTM average volume particle size is 180 nm. It was shown, that the monopropellant's burning rates of the micro- and ultra-sized HMX are almost identical in the pressure range 20 - 100 atm. Two mixing technologies to prepare aluminium/HMX compositions were used: (i) conventional "dry" mixing and (ii) "wet" technique with ultrasonic processing in diethyl ether. BET analysis reveals the highest specific area for composition uHMX/ALEXTM (4.6 m2/g), whereas the lowest one - for the mixture of mHMX/micro-Al (0.5 m2/g). Applying of ultrasonic technique results in a burning rate increase up to 15-20% comparing to "dry" mixing (under initial nitrogen pressure 60 atm). The highest combustion rate was determined for composition of mHMX/ALEXTM (porosity 13%). Influence of component's size and composition's microstructure on the burning rate of energetic systems is discussed and analyzed.

A Study of Sila-Explosives and their Characteistics compared to the Carbon Analogues

Anian Nieder, Thomas M. Klapötke, Burkhard Krumm, Reinhold Tacke, Dennis Troegel

Ludwig-Maximilian University of Munich
University of Würzburg, Institute
of Inorganic Chemistry

anich@cup.uni-muenchen.de, tmk@cup.uni-muenchen.de

Keywords: sila-nitrates; alkyl-nitrates; sila-explosives; sensitivity; crystal structure; NMR.

Recently, the syntheses and characterization of several alkyl and cycloalkyl nitrates have been reported.[1] In the meantime, the corresponding sila analogues were synthesized. These sila derivatives derive from a formal exchange of the quaternary carbon atom of a neopentyl backbone by a silicon atom. The sila analogues were fully characterized by NMR, IR and Raman spectroscopy, and mass spectrometry. Additionally, the sensitivities toward impact and friction were determined. Several of the sila analogues were characterized by single-crystal X-ray diffraction.

Aerobic Biodegradation of 2,4-dinitrotoluene in a Continuous Packed Bed Reactor and Effect of 4-Nitrotoluene Presence

Jan Paca, Martin Halecky, Tereza Hudcova, Evguenii Kozliak

Institute of Chemical Technology
University of North Dakota

jan.paca@vscht.cz, martin.halecky@vscht.cz

Keywords: biodegradation; nitrotoluenes.

Continuous 2,4-dinitrotoluene degradation by a mixed microbial culture immobilized on a porous glass packing material (Poraver) was studied. Experiments were carried out in a packed bed reactor with a counter-current water-air flow under conditions of oxygen in excess. The loading rate was varied by changing the inlet 2,4-DNT concentration at three different water flow rates. The removal efficiency of 2,4-DNT in presence of 4-NT was lower than when 2,4-DNT was degraded as a sole contaminant. The biofilm microbial composition was significantly altered after 3 months of operation. Surface structures of the packing particles and biofilm were characterized using scanning electron microscopy.

An investigation of the influence of inter-phase mechanisms on detonation wave structure

Andrzej Papliński

Military University of Technology

andrzej.paplinski@wat.edu.pl

Keywords: detonation wave structure; non-ideal detonation.

Detonation initiation and evolution of nonstationary detonation wave in air suspensions of combustible droplets is considered. The gaseous suspension of fuel droplets is described as the two-phase medium. Continuous fields of averaged values of mass density, momentum, velocity, internal energy, are introduced. Then, in terms of averaged quantities the balance equations are formulated. The interphase coupling is modelled by introducing the terms of mass, momentum and energy transfer between phases. Strong initiation regime of the detonation process is considered. The initiating shock wave is assumed to arise as a result of explosion of condensed HE charge. Expansion of detonation products are modelled by use of the JWL equation of state. Numerical simulation of the process of evolution of the initiating shock wave and the transition to self-supporting detonation wave is performed. The evaluation are performed by use of a mixed three-step Lagrangean-Eulerian scheme. The half-time step at which the streams and state parameters at the cell borders are estimated is based on a second-order Godunov type scheme. The four-step model of gas-droplet interactions in the process of shock loading is considered. Mass loss due to layer stripping is described by the Engel formula. Evaporation of shattered micro-droplets is modelled in Nusselt approach. The presence of secondary droplets phase arising in the process of primary droplet fragmentation is accounted. The reaction of the gaseous fuel with oxygen from air is described by an overall kinetic scheme. The detailed analysis of the post-shock zone is performed. The influence of the mechanisms of inter-phase coupling: droplets fragmentation and evaporation, energy liberation in fuel combustion upon the shock and detonation wave structure are examined. The placement of the sonic surface, u + c = D is tracking. The resulting split of the relative position of the sonic surface and the end of reaction zone, against the leading shock front is discussed as the example of non-ideal detonation features.

Modeling for Detonation and Energy Release from Peroxides and Non-Ideal Improvised Explosives

Matthew Price, Ang How-Ghee

Energetics Research Institute,
Nanyang Technological University

mattprice@ntu.edu.sg

Keywords: improvised explosives; peroxides; ANFO; non-ideal; reactive flow; air blast.

This work focuses on the development of models for predicting explosive power and air blast from the detonation of organic peroxides (TATP and HMTD) and non-ideal explosives involving ammonium nitrate, urea nitrate, and chlorates. CHEETAH calculations assuming ideal behaviour are in agreement with literature data for peroxides. However, the detonation behaviour of non-ideal explosives is dependent on charge size and confinement. This behaviour is investigated using thermo-chemical calculations with Kinetic CHEETAH, and reactive flow models with AUTODYN. A simplified ignition and growth (I&G) model was calibrated us-ing experimental charge diameter vs. VoD data. I&G models are used to predict the front curvature, reaction zone structure, and energy release from the non-ideal explosives. Detonation and air blast predictions for peroxides and unconfined and confined (paper, plastic, steel) non-ideal charges are presented.

High-pressure structural studies of energetic materials

Colin Pulham, David Millar, Iain Oswald,
William Marshall, Duncan Francis, Adam S. Cumming

The University of Edinburgh
Rutherford Appleton Laboratory
Dstl

c.r.pulham@ed.ac.uk, d.i.a.millar@sms.ed.ac.uk, i.d.h.oswald@ed.ac.uk

Keywords: high pressure; RDX; structure.

The performance of explosive formulations depends on several factors that include crystal density, detonation velocity, and sensitivity to detonation by stimulus. These in turn are governed by the solid-state structure of the energetic material. In order to model and understand the characteristics and performance of these materials, not only under ambient conditions but also under the extreme conditions of temperature and pressure experienced during detonation, it is essential to obtain detailed structural information. This information can be used to explore aspects of energetic materials that include: sensitivity to shock, heat, and friction; chemical decomposition mechanisms; energy transfer through the solid; detonation velocities; and for testing the efficacy of theoretical modelling techniques. Whilst structural information can be readily obtained under ambient conditions, it is much more difficult to obtain at extreme conditions. This presentation will describe how advances in the techniques for the collection and analysis of high-pressure X-ray and neutron diffraction data, in combination with spectroscopic data, now permit the accurate determination of the full crystal structure of energetic materials under extreme conditions. Examples will include two new high-pressure forms of RDX, for which dramatic changes in the conformations of the RDX molecules are observed. Equations of state for both of these forms have also been obtained. Ammonium perchlorate undergoes a first order phase transition at 3.98 GPa in agreement with the results of a previous study. We have successfully solved and refined the structure of the new orthorhombic phase, which features a more close-packed structure with more extensive hydrogen bonding. An equation of state for this new phase up to 8.1 GPa has also been obtained. No evidence was found for a pressure-induced phase transition in ammonium dinitramide up to 4.03 GPa but significant changes were observed in the intermolecular contacts involving N-H...O-N interactions, and in the torsional angles of the dinitramide ion.

Experimental and theoretical studies on structure-properties of some important energetic materials

Yuan-jie Shu, Yajun Luo, Ming Yin, Junliang Du, Xinfeng Wang, Yang Zhou

China Academy of Engineering Physics
Mianyang normal university
Southwest University of Science and Technology

syjfree@sina.com

Keywords: structure; properties; high energy density materials; nitramines; tetrazine; imidazole; pyrazole.

Based on experimental and theoretical studies, effects of structures of some important secondary nitramines on their stability were discussed. Results show that the initial step of decomposition for nitramines is N-NO2 bond dissociation in gas, melt and solid states. The type of nitramine group, conjugation of nitramine with π-electrons and aggregation states are main factors affectting stability of nitramines. New energetic molecules based on tetazine, imidazole and pyrazole were constructed. Their energetic characteristics and thermal stability for tetrazine, imidazole and pyrazole derivatives were studied by means of Quantum chemistry and Molecular mechanics. With these results, some potential candidates of energetic materials were predicted, effects of substitutional groups on properties of these compounds were analyzed. Furthermore, theoretical study of cyclization mechanisms of azide group were carried out. New mechanism was proposed, which may be useful for synthesis of azide compounds.

Azidotetrazoles – Promising Energetic Materials or Waste of Time?

Jörg Stierstorfer, Thomas M. Klapötke, Stefan Sproll, Franz A. Martin

Ludwig-Maximilian University of Munich

jstch@cup.uni-muenchen.de

Keywords: energetic materials; tetrazoles; azides; X-ray; detonation parameters; sensitivity.

Several new 5-azidotetrazoles, such as 1-methyl-5-azidotetrazole, 2-methyl-5-azidotetrazole, 1,2-bis(5-azidotetrazolyl)ethane, 1,2-bis(5-azidotetrazolyl)propane, 1,2-bis(5-azidotetrazolyl)-butane and 1-(2-azidoethyl)-5-azidotetrazole were synthesized by different synthetic routes. All compounds have been characterized comprehensively by low temperature X-ray diffraction, IR, Raman and NMR spectroscopy, mass spectrometry and differential scanning calorimetry. The heats of formation have been calculated by the atomization energy method yielding highly endothermic values. With these and the X-ray densities several detonation parameters such as the explosion energy as well as the detonation pressure and velocity have been computed using the EXPLO5 software. In addition the impact, friction and electrical spark sensitivity of all compounds have been explored by the BAM drophammer, friction tester and an OZM small scale electrical discharge device. Last but not least, the results have been concluded and classified regarding the use of 5-azidotetrazoles in energetic applications.

Synthesis of 1H-benzo[d]imidazol-2(3H)-one polynitroderivatives

Ekaterina Tatarnikova, Vladimir Sizov, Igor V. Tselinsky, Aleksandr Aleksandrov

Saint-Petersburg State Institute of Technology

sizek@list.ru

Keywords: synthesis; nitration; benzimidazole-2-one; rearrangement.

N-Nitroderivatives of 1H-benzo[d]imidazol-2(3H)-one: 1,5,6-trinitro-, 1,3,5,6-tetranitro- and 1,4,5,6-tetranitro-1H-benzo[d]imidazol-2(3H)-ones were first synthesized by nitration of 5,6-di- and 4,5,6-trinitro-1H-benzo[d]imidazol-2(3H)-one with nitric acid in acetic anhydride. The rearrangement of N-nitrobenzimidazolones under heating in various solvents (ethylacetate, buthylacetate, acetonitrile, acethone, dioxan, o-dichlorobenzole, anizole) into C-nitroderivatives was studied. The method for 4,5,6,7-tetranitro-1H-benzo[d]imidazol-2(3H)-one synthesis by nitration of 1H-benzo[d]imidazol-2(3H)-one, 5,6-di- and 4,5,6-trinitro-1H-benzo[d]imidazol-2(3H)-ones with low excess of nitric acid in acetic anhydride at 50-60oC was developed based on facility of the rearrangement process. Tetranitroderivative was obtained in 85-90% yield. The preparation procedure of 4,5,6-trinitro-1H-benzo[d]imidazol-2(3H)-one via nitration of 1H-benzo[d]imidazol-2(3H)-one and 5,6-dinitro-1H-benzo[d]imidazol-2(3H)-one in sulfuric acid with nitric acid taken in 1.5-fold excess was suggested. 4,5,6,7-Tetranitro-1H-benzo[d]imidazol-2(3H)-one was synthesized in 81% yield in a similar manner by nitration of 4,5,6-trinitro-1H-benzo[d]imidazol-2(3H)-one.

Standoff Explosives Detection Technologies - An Overview

Sara Wallin Wallin, Anna Pettersson

FOI, Swedish Defence Research Agency

sara.wallin@foi.se

Keywords: standoff; detection; explosives.

A review of standoff detection technologies for explosives has been made. The re-view is limited to trace detection methods (methods aiming to detect traces from handling explosives or the vapours surrounding a charge due to the vapour pres-sure of the explosive) rather than bulk detection methods (methods aiming to detect the bulk explosive charge). The requirements for standoff detection technologies are discussed. The technologies discussed are all laser based technologies, such as Laser-Induced Breakdown Spectroscopy (LIBS), Raman, Laser-Induced Fluores-cence (LIF) and IR spectroscopies. The review includes novel techniques, not yet tested in realistic environments as well as more mature technologies which have been tested outdoor in realistic environments.

Artificial Neural Networks in Energetic Materials Enthalpy of Formation Calculations

Nelly Zhokhova, Tatyana Pivina, Lyubov Maslova, Yuriy Matyushin, Alexey Zefirov

M. V. Lomonosov Moscow State University
Zelinsky Institute of Organic Chemistry, Russian Academy of Siences
Zelinsky Institute of Organic Chemistry, Russian Academy of Siences
Semenov Institute of Chemical Physics, Russian Academy of Siences
M. V. Lomonosov Moscow State University

zhokhova@org.chem.msu.ru, tsp@ioc.ac.ru

Keywords: artificial neural networks; QSPR; enthalpy of formation.

The enthalpy of formation is one of the most important properties for energetic ma-terials. Using method of Quantitative Structure–Property Relationships (QSPR), such as Artificial Neural Networks (ANN), attempts to investigate structure–enthalpy of formation relationships for a certain database are made and models for estimation and prediction of this characteristic are elaborated.

Pre-explosive Emission of Electrons from Silver Azide

**Edward Aluker, Alexander Krechetov, Anatoliy Mitrofanov,
Alexander Pashpekin, Alexander Samarov**

Kemerovo State University
Kemerovo Department of the Institute of Solid-State
Chemistry and Mechanochemistry SB RAS

lira@kemsu.ru, kag@kemsu.ru

Keywords: silver azide; pre-explosive phenomena; electron emission.

A new phenomenon of preexplosion electron emission from energetic materials was experimentally was revealed, a process that accompanies initial stages of explosive decomposition in the solid phase, before the onset of intense energy release and sample dispersion.

Temperature Dependencies of Laser Initiation of PETN

Edward Aluker, Alexander Krechetov, Denis Nurmukhametov, Alexander Tupitsyn

Kemerovo State University
Kemerovo Department of the Institute of Solid-State
Chemistry and Mechanochemistry SB RAS

lira@kemsu.ru, kag@kemsu.ru

Keywords: PETN; laser initiation.

The temperature dependence of the probability of PETN explosion upon laser pulse initiation (1064 nm, 10 ns, 1–5 J) was examined. As the temperature increases from 393 K to 450 K, the initiation threshold lowers, with the initiation of open-surface samples occurring over the entire temperature range. It was concluded that the initiation mechanism involves thermal-and photoactivation steps. The activation energy for the thermal activation step was found to be 0.35 ± 0.05 eV.

The energetically aspects of the physical and chemical processes in conditions -high pressure + shift

Khachatur A. Arutyunyan, Yuri M. Burov, Lyudmila V. Pletneva, Valentin D. Tshepilov

Institute of Problems of Chemical Physics RAS
Experimental Factory Scientific Engineering and Special Design of RAS
Peoples' Friendship Universities of Russia

Keywords: high pressure + shift; polymerization; mixture; Bridzhmens anvil.

The considerable quantity of mechanical energy can be entered into substance in conditions "high pressure + shift". The density of this energy can surpass on usages density of chemical energy in the energetic materials. This energy can cause the various processes similar to processes. These processes are similar to the processes which are occurring in shock waves. It is possible to tell that processes in conditions "high pressure + shift" are static model the shock waves phenomena. Thus unlike shock waves the processes "high pressure + shift" occur in the much softer, controllable conditions. It facilitates their studying. In the present work the results of research of two processes which occur in conditions "high pressure + shift", and in shock waves are presented: polymerization of the monomer and mixture thermodynamically incompatible polymers.

Impact sensitivity of nitrimines

Alexander M. Astachov, Vitaliy A. Revenko, Eduard S. Buka

Siberian State Technological University

alexastachov@mail.ru

Keywords: energetic compounds; nitrimines; impact sensitivity.

Impact sensitivity (drop-hummer machine K-44-II) of nitrimines (energetic compounds containing explosophoric molecular fragment >C=N-NO2) are considered in the present work. Contrary to data of the separate publications claiming about low level of sensitivity of the some nitrimines, in the present work it is shown that considered compounds are high-sensitivity explosives in the majority cases. It is revealed that presence in nitrimines crystallyzation water not only does not lead to lowering sensitivity of nitrimines but on the contrary promotes initiation of explosion at impact. Observable experimental data are considered from the point of view of the classical thermal theory of initiation of explosion by mechanical impact and they explained through the mechanism of thermal decomposition of nitrimines.

The crystal and molecular structure of 3-nitro-1-trinitromethyl-1,2,4-triazole

Alexander M. Astachov, Alexander D. Vasiliev, Andrew A. Erashov, Ludmila A. Kruglyakova, Rudolf S. Stepanov

Siberian State Technological University
Institute of Physics RAS (Siberian branch)

alexastachov@mail.ru

Keywords: high explosives; nitrocompounds; 1,2,4-triazole; X-ray structure.

The 3-nitro-1-trinitromethyl-1,2,4-triazole (NTNMT) structure was solved by X-ray methods. Crystals of NTNMT possess the monoclinic system, space group P21/c, with cell parameters: a = 6.658(7)A.U., b = 20.56(2)A.U., c = 6.730(7)A.U., b = 94.22(1)degree, Z = 4, V = 919(3)A.U., dx-ray = 1.901 g/cm3. The molecule contains planar nitro-1,2,4-triazole group and trinitromethyl fragment with tetrahedral conformation of carbon atom.

The investigation of the interaction of 2,4,6-trichloro-1,3,5-triazine with salts of gem-dinitrocompounds

Vladimir V. Bakharev, Alexander A. Gidaspov,
Vladimir A. Zalomlenkov, Eugene A. Kozhevnikov

Samara State Technical University

knil@sstu.smr.ru

Keywords: 2,4,6-trichloro-1,3,5-triazine; salts of gem-dinitrocompounds; dinitromethylation.

The approach to the synthesis of dinitromethyl derivatives of 1,3,5-triazine based on the interaction of 2,4,6-trichloro-1,3,5-triazine with different aliphatic dinirocompounds salts (chloro-, fluorodinitromethane, dinitroethane, dinitroethanol, ethyl dinitroacetate, dinitroacetonitrile) was studied. It's shown the outcome of reactions is dependent on the nature of the substituent on the dinitromethyl carbon.

Investigation of Products and Velocity of Detonation of „Improvised Explosive Filler”

Nadja Barl, Thomas M. Klapötke, Burkhard Krumm, Susanne Scheutzow, Franz Xaver Steemann

Ludwig-Maximilian University of Munich

Keywords: improvised explosives; detonation velocity.

Improvised Explosive Devices impose a considerable threat upon military as well as civilians. Analytical data of the detonation products and traces of improvised explosive devices can serve criminal investigations. Performance data of the devices can aid in the construction of fortification and protection of buildings. As example for a widely known improvised explosive, "improvised explosive filler" was prepared and detonated inside a detonation chamber. The detonation velocity was measured and the residues on the inner surface of the chamber was recovered and investigated.

The effect of different additives on the explosive behaviour of composition B

Sameh Basuony, Hosam Mostafa, Mohamed Seleet

Egyptian Armed Forces

samehbsn@yahoo.com

Keywords: composition B mixtures; sensitivity; gap test; differential scanning calorimetry; decomposition.

Composition B, which is an explosive mixture of RDX and TNT, is used as the destructive charge in artillery shells, rockets and landmines. Several researches discussed the enhancement of the performance and safety aspects of this explosive. In this paper composition B mixtures with Aluminum (as an active metallic additive) and Polyurethane (as an inert polymeric binder) were prepared and characterized. The sensitivity of the prepared formulations towards different initial impulses as heat, friction and shock wave was markedly dependent on the additive type. Polyurethane-based composition was found to have the lowest sensitivity to friction; composition B has the lowest sensitivity to shockwave while Aluminum-based composition has the lowest sensitivity to heat. Differential Scanning Calorimetry (DSC) experiments and the activation energy calculations of the decomposition step for the prepared formulations showed that the Polyurethane-based composition decomposes at lower temperature than the other formulation.

Identification of alpha-chloro-2,2',4,4',6,6'-hexanitrobibenzyl as an impurity in hexanitrostilbene (HNS)

Anthony J. Bellamy

Cranfield University

a.j.bellamy@cranfield.ac.uk

Keywords: HNS; hexanitrostilbene.

The final intermediate in the Shipp synthesis of HNS from TNT, alpha-chloro-2,2',4,4',6,6'-hexanitrobibenzyl, has been extracted and characterised by NMR spectroscopy, elemental analysis and HPLC. It has also been shown that digestion in NMP of HNS containing alpha-chlorohexanitrobibenzyl, generates another chlorine-containing by-product, 2-chloro-2',4,4',6,6'-pentanitrostilbene. This too has been characterised by NMR spectroscopy, elemental analysis and HPLC.

Crystal habit of LLM-105 (2,6-diamino-3,5-dinitropyrazine 1-oxide)

Anthony J. Bellamy, Peter Golding, Mary Mahon

Cranfield University
AWE Aldermaston
University of Bath

a.j.bellamy@cranfield.ac.uk

Keywords: LLM-105; 2,6-diamino-3,5-dinitropyrazine 1-oxide; morphology.

LLM-105 (2,6-diamino-3,5-dinitropyrazine 1-oxide) when synthesised by oxidation of 2,6-diamino-3,5-dinitropyrazine i.e. separation from H2O2/CF3COOH, crystallises as compact blocks, or even needles when a co solvent is present. However when it is synthesised by nitration of 2,6 diaminopyrazine 1-oxide i.e. crash precipitation with water from mixed acid, it crystallises as leaf- or fern-like plates. Similarly when LLM-105 is crash precipitated from H2SO4 solution, it also crystallises as leaf- or fern-like plates. These various crystal habits have been examined by powder XRD and shown to have the same morphology as that reported by Gilardi and Butcher [4] for 2,6 diamino-3,5-dinitropyrazine 1-oxide.

New energetic polymers based on cellulose

Franziska Betzler, Thomas M. Klapötke, Stefan Sproll

Ludwig-Maximilian University of Munich

fbech@cup.uni-muenchen.de

Keywords: cellulose; energetic polymer; nitrogen rich polymer; tetrazole.

New energetic polymers based on cellulose were synthesized using common procedures. The point of interest was the introduction of tetrazole containing moieties. The polymers were characterized by vibrational spectroscopy (IR). The energetic properties of the polymers were investigated using differential scanning calorimetry and bomb calorimetric measurements along with calculations using the EXPLO5 software.

Analysis of terminal effectiveness for several types of HE projectiles and impact angles using numerical-CAD technique

Alan Catovic, Berko Zecevic, Jasmin Terzic

University of Sarajevo, Mechanical Engineering
Faculty, Defense Technologies Department

Keywords: natural fragmentation; lethal zones; HE projectiles.

Important task of HE projectile terminal ballistics is determination of lethal area. Lethal area is a measure of fragment casualty-producing potential of an exploding projectile when employed against human targets, and can be expressed as a function of soldiers density and probability that the personnel will be incapacitated. Researchers worldwide use different criteria for human target densities. It means that expected number of casualties (physical meaning of lethal area, according to US model), after detonation of single projectile, will strongly depend on chosen criteria for soldiers density on terrain.

In our model, based primarily on U.S. Vulnerability Model, lethal zone of HE warheads is defined as a zone on the battlefield in which an efficient fragment density is greater or equal to 1 frag/m2. That means that the Isodensity curve, a curve which connects points with the same efficient fragment density, presents an envelope of HE warhead lethal zone. Soldiers standing inside of this lethal zone presumably will be incapacitated by an efficient fragment hit. It is important to note that data for fragment densities are obtained from experimental test in Arena facilities.

In order to perform analysis of terminal effectiveness for different types of HE projectiles and their impact angles, alternative approach with CAD technique was introduced. Using spline interpolation and 3D technique in CAD software, it is possible to predict 3D model of lethal zones for HE projectiles. Rotating and mirroring these 3D models in space helps us in determination of HE projectile attack angle influence on its lethal zone. Furthermore, using intersection CAD technique for obtained 3D models, 2D model of lethal zones can be obtained for different attack angles and different presented area of soldiers on terrain. Areas of obtained 2D models can be easily determined in CAD software. These lethal zone areas are great visual and intuitive tool for analysis of terminal effectiveness of HE projectile.

On the reaction of NTO (3-nitro-1,2,4-triazol-5-one) and FOX-7 (1,1-diamino-2,2-dinitroethene) with alkyl isocyanates

Alessandro Contini, Anthony J. Bellamy, Matt Andrews

Cranfield University

a.contini@cranfield.ac.uk

Keywords: 3-nitro-1,2,4-triazol-5-one; 1,1-diamino-2,2-dinitroethene.

The reactivity of the less-sensitive explosives NTO (3-nitro-1,2,4-triazol-5-one) and FOX-7 (1,1-diamino-2,2-dinitroethene) towards simple alkyl isocyanates was investigated. New carboxamidic derivatives have been synthesised by reacting the explosives with 1-isocyanatohexane (NTO and FOX-7) and 1,6-diisocyanatohexane (NTO only) under relatively mild conditions. The new products were characterised by a combination of 1H and 13C NMR and FTIR spectroscopy, single crystal X-ray diffraction and differential scanning calorimetry.

The influence of molybdenum and titanium on selected properties of high calorific Fe-$KClO_4$ mixture

Bogdan Czajka, Leszek Wachowski, Zenon Foltynowicz, Katarzyna Lipinska, Marek Lipinski, Stanislaw Tabat

Institute of Non-ferrous Metals Branch in Poznan
Adam Mickiewicz University
University of Economics
MESKO Metal Works S.A.
MESKO Metal Works S.A.
Institute of Non-ferrous Metals Branch in Poznan

bogdan.czajka_xl@wp.pl, wachow@amu.edu.pl, zenon.foltynowicz@ae.poznan.pl

Keywords: Fe-$KClO_4$ mixture; activators; burning rate; specific calorific value; mechanical properties; test stability.

Appropriately prepared ingredients of a high calorific mixture containing potas-sium chlorate(VII), iron powders of various origin and selected metallic powders (Mo and Ti) used as activators were investigated. It has been established that burn rate of the investigated calorific mixture depends on the presence of activator (in-troduced in the amount in the range of 1-5 wt.%) and increased in the following order: Ti>Mo. Thermal effect was higher in comparison to the parent mixture, too.

Linear Shaped Charge With Emulsion Explosive

Mario Dobrilović

University of zagreb, Faculty of mining,
geology and petroleum engineering

mardob@rgn.hr

Keywords: emulsion explosive; linear shaped charge; jet velocity.

Research program and results of program testing and measurements performed with linear shaped charge with emulsion explosive are described in paper. Linear shaped charges that are available on the market include high monomolecular explosive with high detonation velocities like RDX or PETN for jet formation. Efficient of that charges is confirmed but price of that explosives raises cost of linear shaped charge. Researches and tests that have been carried out in Laboratory for testing of civil explosives, Faculty of mining, geology and petroleum engineering, Zagreb, on the linear shaped charge with emulsion explosive. Those researches have proved function and efficiency of that kind of liner. Tests were carried out with two kind of emulsion linear shaped charge: for lined cuts and for cuts of cylindrical steel bodies like pipes. Cutters construction during testing was varied with charge mass, angle and stand off. For comparative purposes, type of explosive and material of liner were changed. Measurement of velocity of detonation of explosive and liner jet velocity have been done. According to test and measurements during the research program, function of shaped liner charge with emulsion explosive was proved with different construction parameters.

Synthesis of di- and trinitropyrazoles

Stefan Ek, Nikolaj Latypov, Grégoire Hervé, Guy Jacob, Patrick Goede

Swedish Defence Research Agency (FOI)
SNPE Matériaux Energétiques

stefan.ek@foi.se, nikolaj.latypov@foi.se

Keywords: synthesis; nitropyrazoles; energetic materials.

Pyrazole derivatives are promising as new low sensitivity energetic materials, due to the pyrazole nucleus, which offers numerous synthetical possibilities together with a relatively high heat of formation. Therefore, several members of the nitropyrazole series were synthesised and the more promising out of these were characterised.

In this paper, new synthesis methods for two trinitropyrazoles, several dinitropyrazoles and some of their characteristics are described. 3,4,5-trinitropyrazole was synthesised in two different ways. The other trinitropyrazole, namely the 1,3,4-trinitroisomer, was used as an intermediate in the synthesis of 5-amino-3,4-dinitropyrazole. This latter compound could also be oxidised into 3,4,5-trinitropyrazole.

Explosive Properties Effect on the Performance Characteristics of Shaped Charges

Tamer Elshenawy

Egyptian Armed Forces

tamershenawy@yahoo.com

Keywords: shaped charge; AUTODYN; explosives.

Chemical energy or shaped charge is considered one of the more important penetration capabilities of armors in the main battle tank as well hard Rocks in oil well perforators used in oil industry. In this paper, a series of computer simulation models using Ansys-Autodyn hydrocode were performed in order to investigate the produced jet characteristics and predicted penetration capabilities by using different types of explosives in the main charge of small caliber shaped charge of 30mm base diameter and electrolytic Cupper for trumpet shape liner. Also the wave shaper or wave former design inside the main explosive sharge is considered during the analysis of the output data fom the code.

The analysis models of selected shaped charges using Autodyn-3D hydrocde involves the shaped charge jetting analysis, jet formation profiles, jet tip velocities, cumulative jet masses and selected gauge points characteristics, (pressure, compressibility, stresses,. . . . .).

The output data are analyzed using virtual origin model and penetration depth equation models for both continuous and particulized jet. The penetration results based on these models are compared with that obtained by Autodyn hydrocode.

Means of initiation and velocity of detonation of ANFO explosives

Zvonimir Ester

Faculty of mining geology
and petroleum engineering

zvonimir.ester@rgn.hr

Keywords: initiation; velocity of detonation; ANFO.

For the explosives mixed on the field of use, laboratory testing of their characteristic can not be done in advance. VOD velocity of detonation, measured in blast hole is cheap and simple method that ensure determination of explosive properties, in situ. ANFO can be initiated with appropriate booster or with small charge of some other explosive that is sensitive to impulse of detonator cap no. 8. Initiations of blast holes charges were conducted in different ways with three different explosives and velocity of detonation measurements results are compared in paper. Measurements purpose was to bring optimal mean of initiation respecting economy and technical factors.

Applicability of thermal methods for determination of nitroglycerine content in double based propellants

Ivona Fiamengo, Muhamed Sućeska, Sanja Matečić Mušanić

Brodarski institut-Marine Research
& Advanced Technologies

Keywords: thermal methods; thermogravimetry; identification; homogeneous propellants; double based propellants; nitroglycerine.

Thermal methods play important role among various measuring technique used in the analysis of explosive materials. These methods are mostly used for the investigation and determination of thermal properties of energetic materials (e.g. melting process, polymorphic transformations, temperature of initiation, etc.), as well as to estimate thermal stability, and to study thermal decomposition. Furthermore, thermal methods can be also used for analytical purposes, such as identification of some commonly used high explosives, determination of their purity, determination of phlegmatiser content, etc. The aim of this work was to study the possibility of isothermal and non-isothermal thermogravimetry (TGA) application for identification of the homogeneous propellants type, and to determine nitroglycerine content in double based propellants. It has been found out from the shapes of TGA thermograms, i.e. from the position of some characteristic points on the theromograms that it is possible to distinguish clearly between nitrocellulose and double based propellants. Furthermore, from the isothermal and non isothermal TGA thermograms, nitroglycerine content in double based propellants could be roughly determined (with an error less than 5%).

Increasing the Nitrogen Content of Single-Base Propellant Elements

Svetlozar Ganev, Radi Ganev

University of Chemical Technology and Metallurgy
Civil Engineering Higher
School (VSU) Luben Karavelov

radiganev@abv.bg, radiganev@abv.bg

Keywords: propellants; nitrogen content; UV spectroscopy.

Processes of deposition of trotyl, tetryl and ammonium nitrate on elements made of nitrocellulose (NC) by means of diffusion and surface application were investigated. The adsorption processes were examined with ultraviolet (UV) spectroscopy, and the time for the course of those processes was established. It has been established that the UV spectroscopy (UVS) is not suitable for examining the processes of diffusion of the tetryl in single-base propellants. The calorimetric investigations show the advantages of the modification of the single-base propellants by means of adsorption.

The fluoration of dinitromethyl-1,3,5-triazine salts with xenon difluoride

Alexander A. Gidaspov, Vladimir V. Bakharev, Elena V. Velikanova, Igor V. Tselinsky

Samara State Technical University
Saint-Petersburg State Institute of Technology

knil@sstu.smr.ru, knil@sstu.smr.ru

Keywords: dinitromethyl-1,3,5-triazine salts; xenon difluoride; fluorodinitromethyl-1,3,5-triazines.

The substances containing fluorodinitromethyl functionality are attracting interest as low sensitive high explosives and energetic plasticizers. Fluorodinitromethyl-1,3,5-triazines are relatively unexplored class of compounds. The known methods of their synthesis are based on cyclotrimerization of fluorodinitroacetonitrile or on interaction of non stable fluorodinitromethane salts with 2,4,6-trichloro-1,3,5-triazine. The synthesis of fluorodinitrometyl-1,3,5-triazines via the interaction of dinitromethyl-1,3,5-triazine with soft fluoration agent (xenon difluoride) was developed

Replacement of RDX and HMX: BTAT, a structural isomer of CL-20

Michael Göbel, Thomas M. Klapötke

Ludwig-Maximilian University of Munich

Keywords: BTAT; high performance explosive.

BTAT, N3,N6-bis(2,2,2-trinitroethyl)-1,2,4,5-tetrazine-3,6-diamine, has been synthesized and comprehensively analyzed including multinuclear NMR spectroscopy, IR and Raman spectroscopy, high resolution mass spectrometry, elemental analysis and differential scanning calorimetry and x-ray crystallography. Energetic sensitivity data have been experimentally determined (impact, friction, electrostatic sensitivity) or theoretically calculated (heat of formation, performance properties).

Replacement of TNT: BTHC, an insensitive melt castable explosive with positive oxygen balance

Michael Göbel, Thomas M. Klapötke

Ludwig-Maximilian University of Munich

Keywords: HOX; melt castable explosive.

BTHC, bis(2,2,2-trinitroethyl)-hydrazodicarboxylate, has been synthesized and comprehensively analyzed including multinuclear NMR spectroscopy, IR and Raman spectroscopy, high resolution mass spectrometry, elemental analysis and differential scanning calorimetry and x-ray crystallography. Energetic sensitivity data have been experimentally determined (impact, friction, electrostatic sensitivity) or theoretically calculated (heat of formation, performance properties).

New energetic materials based on 2H-tetrazole-5-carboxylic acid

Vera Hartdegen, Thomas M. Klapötke, Stefan Sproll

Ludwig-Maximilian University of Munich

Keywords: 2H-tetrazole-5-carboxylic acid; tetrazole; energetic; nitrogen rich.

Several new energetic compounds based on 2H-tetrazole-5-carboxylic acid were synthesized. All compounds were characterized by vibrational spectroscopy (IR), mass spectrometry and multinuclear NMR spectroscopy. The crystal structures of the compounds were determined using single crystal X-ray diffraction. In addition the thermal behavior of the compounds was monitored using differential scanning calorimetry.

Size/strain diffraction peak broadening of the energetic materials RDX, ADN and FOX-7

Michael Herrmann, Ulrich Förter-Barth, Paul Bernd Kempa

Fraunhofer Institut Chemische Technologie

michael.herrmann@ict.fraunhofer.de

Keywords: X-ray diffraction; microstructure; energetic materials.

X-ray powder diffraction is an established tool for the investigation of energetic materials. The positions and intensities of diffraction peaks yield information of the crystal structure described by the dimensions and the internal structure of the elementary cell. Thus they are used for investigations of, e.g., polymorphism, phase transitions, crystal density, thermal expansion and residual strain. Further information is available from the peak profiles which are related to the real structure described by crystallite size, shape and micro strain. The last represents lattice distortions or imperfections as impurities, twins, dislocations, grain boundaries, misfits or stacking faults. A series of energetic materials have been measured at the synchrotron ANKA, amongst them RDX, HMX, ADN, CL-20, FOX-7 and FOX-12. The results have been evaluated by means of Williamson-Hall-plot and a double Voigt Approach implemented in the Program TOPAS from Bruker AXS. Characteristic line broadening was found for these materials and in case of HMX and RDX different qualities are investigated. The presentation shows results of RDX, ADN and FOX-7.

Reaction of methylnitramine and ethylenedinitramine with dihalogenmethanes

Zdeněk Jalový, Jaromír Foud

University of Pardubice

Keywords: 2,4-dinitro-2,4-diazapentane; dibromomethane; bromochloromethane; 1,3-dinitroimidazolidine.

Methylnitramine (1) reacts with dibromomethane (2a) or bromochloromethane (2b) in the presence of potassium carbonate as a base to produce 2,4-dinitro-2,4-diazapentane (3) in the yields of 28 % and 23 %, respectively. When ethylenedinitramine (4) reacts with dihalogenmethanes at the same conditions, 1,3- dinitroimidazolidine (5) is formed. However, the yield of 5 is considerably lower than in the case of 3.

1-(1,1-Dihydroperfluoroalkyl)-5-perfluoroalkyl tetrazoles

Konstantin Karaghiosoff, Thomas M. Klapötke, Hendrik Radies

Ludwig-Maximilian University of Munich

klk@cup.uni-muenchen.de

Keywords: 1,1-dihydroperfluoroaklyl azide; disubstituted fluorinated tetrazoles.

A series of 1H,1H-perfluoroaklyl azides were synthesized from 1H,1H-perfluoroalkan-1-ols via metathesis reactions using 1H,1H-perfluoroalkyl tosylates or mesylates. The azides were characterized using vibrational (infrared) and multinuclear NMR spectroscopy, differential scanning calorimetry, elemental analysis, and mass spectrometry. In addition, the reactions of the azides with perfluoroalkyl nitriles to the fluorinated tetrazoles were carried out.

Crystallization of RDX with an Internal Seeding Technique for Reduction of Solvent Inclusion

Junwoo Kim, Jae-Kyeong Kim, Hyoun-Soo Kim, Kee-Kahb Koo

Sogang University
Agency for Defense Development

marostyle@sogang.ac.kr, tetrapodfish@empal.com

Keywords: RDX; inclusion; internal seeding.

One focus of the current research in high-energetic materials such as RDX (cyclotrimethylene-trinitramine) and HMX (cyclotetramethylene-tetranitramine) is reduction of shock sensitivity by controlling the crystal defects such as liquid inclusion. In the present work, from quantitative analysis on crystal growth rate and amount of solvent inclusion and image analysis of RDX crystals by SEM, large amount of solvent was found to be included at initial crystal growth period. Considerable reduction of liquid inclusion in RDX crystals was found to be possible by the internal seeding technique. Optimum condition of the internal seeding technique was determined by quantitative analysis on crystal size distribution and amount of solvent included in RDX crystals.

Preparation and Properties of Energetic Trimethylamine Derivatives

Thomas M. Klapötke, Burkhard Krumm, Mathias Scherr, Franz Xaver Steemann

Ludwig-Maximilian University of Munich

Keywords: trimethylamine derivatives; tris(chloromethyl)amine; tris(5-nitrotetrazol-2-ylmethyl)amine; tris(azidomethyl)amine.

Tris-(5-nitrotetrazol-2-ylmethyl)amine was prepared and fully characterized using DSC, bomb calorimetry, as well as vibrational, multinuclear NMR spectroscopy, and X-ray diffraction. Its properties were compared with the very energetic tris(azidomethyl)amine and displayed significant lower sensibilities. The structure of tris(azidomethyl)amine was calculated at the B3LYP/6-31G(d) level of theory.

Insensitive Explosives and Propellants Based On 1,2,4-Oxadiazol Derivatives

Thomas M. Klapötke, Martin H. Kunzmann, Norbert T. Mayr, Stephanie Seel

Ludwig-Maximilian University of Munich

tmk@cup.lmu.de

Keywords: propellants; explosives; energetic salt; nitrogen rich; oxadiazol; dinitramide; picrate; guanidine.

The aims of research for new explosives are a better or equal performance to RDX, safety in handling, a high temperature and longterm stability and also a low toxicity. These necessary properties are accomplished by the class of oxadiazol derivatives. The most common compound for explosives are the 1,2,5-oxadiazol derivatives (furazanes) which have high performance but often a lack of stability. The 1,2,4-oxadiazol derivatives are combined with a selection of energetic synthons. The nitrogen rich bis-1,2,4-oxadiazol-5-onate salts show interesting properties as propellants.

Smokeless Pyrotechnical Colorants Based On 1,2,4-Oxadiazol-5-onate Salts

Thomas M. Klapötke, Norbert T. Mayr, Stephanie Seel

Ludwig-Maximilian University of Munich

tmk@cup.lmu.de

Keywords: pyrotechnics; colorant; energetic salt; strontium; copper; lithium; oxadiazol; crystal structure.

Pyrotechnical compositions are created from polymeric binders, oxidizers and colorants. For bright and illuminating fireworks this colorants need to be of high color purity and bare smokeless combustion. Especially in commercial fireworks as in theme parks or during holiday celebrations used there should be also low toxicity. The class of colorful bis-1,2,4- oxadiazol-5-onate salts fulfills these requirements in a very good way. The copper salts show a saturated green color and the lithium and strontium salts a very shiny red color. The toxicity was reduced through the exchange of the commonly used perchlorate anion.

Energetic Salts of Low Symmetry Methylated 5-Aminotetrazoles

Thomas M. Klapötke, Carles Miró Sabaté

Ludwig-Maximilian University of Munich

tmk@cup.uni-muenchen.de

Keywords: density functional calculations (DFC); energetic materials; heterocycles; secondary interactions; X-ray structures.

Ionic salts containing the novel 2-methyl-5-aminotetrazolium and 1,3-dimethyl-5-aminotetrazolium cations with energetic anions (perchlorate, nitrate, azide and dinitramide) were synthesized in high yields and purities and fully characterized. A full structural description by means of spectroscopic methods (vibrational and 15N NMR spectroscopy) and X-ray analysis is given here. Unexpectedly, salts based on the asymmetric 1,3-dimethyl-5-aminotetrazolium cation have higher densities than analogue compounds containing the isomeric 1,4-dimethyl-5-aminotetrazolium cation, regardless of the lower symmetry of the former. This can be attributed to secondary interactions between cation and anion and is reflected in the higher detonation parameters of the new compounds, which represent a new class of nitrogen-rich, high-performing materials with low sensitivity and promise for energetic applications.

Pyrotechnics, Propellants and Explosives: Bridged 5-Nitrotetrazole Derivatives

Thomas M. Klapötke, Carles Miró Sabaté, Matthias Rasp

Ludwig-Maximilian University of Munich

Keywords: energetic; nitrogen rich; heterocycles; laser induction; X-ray structures.

An improved procedure for the synthesis of ammonium 5-nitrotetrazolate (ANT) is given here, which allows to prepare the material on a large scale. ANT was selectively alkylated with bromoacetonitrile yielding 5-nitrotetrazole-2-ylacetonitrile (NTAN). The 1,3-dipolar cycloaddition of NTAN rendered 5-(5-nitrotetrazole-2-ylmethyl)-tetrazole (NTTz). A family of energetic salts based on the novel 5-(5-nitrotetrazole-2-ylmethyl)-tetrazolate anion (NTTz–) with alkali (Li+, Na+, K+, Rb+ and Cs+) and transition (Cu2+ and Ag+) metals and ammonium and guanidium cations were synthesized. All new compounds were characterized by analytical (elemental analysis and mass spectrocometry) and spectroscopical methods (IR, Raman and NMR spectroscopy) and the crystal structures of the NTTz– anion in some of the compounds was solved by means of low temperature X-ray diffraction analysis. Due to the interest of tetrazole derivatives as energetic materials, the sensitivities and energetic properties of all compounds to friction and impact were determined. Some of the metal salts show promise as primary explosives and, interestingly, the silver and copper salts are easily and safely initiated by the laser beam generated by a Raman machine. On the other hand, the nitrogen-rich salts exhibit high detonation pressures and velocities. Most of the compounds have good thermal and chemical stability and are potential candidates for application as environmentally friendly pyrotechnics, propellants or explosives.

Salts of 1-(2-Chloroethyl)-5-Nitriminotetrazole – New Candidates for Coloring Agents in Pyrotechnic Compositions

Thomas M. Klapötke, Jörg Stierstorfer, Karina R. Tarantik

Ludwig-Maximilian University of Munich

Keywords: pyrotechnics; nitriminotetrazolates; coloring agent; perchlorate-free.

Alkaline and alkaline earth metal salts are widely used in pyrotechnic formulations as colorant agents. Sodium salts, for example Na2C2O4, are inserted to yield a yellow flame color. Salts of lithium or strontium are responsible for a red one, barium salts, mostly Ba(NO3)2, for a green flame color and copper salts, only combined with a chlorine donor, are able to yield a blue flame color. Therefore, the lithium, sodium, potassium, calcium, strontium and barium salts of 1-(2-chloroethyl)-5-nitriminotetrazole and diaqua copper(II) 1-(2-chloroethyl)-5-nitriminotetrazolate dihydrate were synthesized and characterized using vibrational and NMR spectroscopy, elemental analysis, and differential scanning calorimetry (DSC). Their sensitivities towards shock, friction, and electrostatic sparks were determined and the heats of formation were calculated using bomb calorimetric measurements. Crystal structures have been determined by single crystal X-ray diffraction. Last but not least, all salts were tested with regard to their color performance in different pyrotechnic compositions.

Characteristics of Sensitivity to Impact Ammonium Perchlorate and Its Composition with Al and Al_2O_3

Denis Kokovikhin, Alexander Dubovik

Mendelejev University of Chemical Technology

deniskokovikhin@mail.ru

Keywords: sensitivity to impact; ammonium perchlorate; aluminium powder.

The method of critical energies (CE) were used for detection sensitivity to impact of solid binary compositions on the basis of ammonium perchorate (AP), including sensitivity one. In this work were used ultrafine powder of AP (d=2-20 micron), aluminium of mark PAP-2 (d=0,2 - 5 micron) and powdery aluminium oxide (corundum). Besides, experiment with composition containing nanoaluminium and nano-AP were carry out. All tests were put on drop-weight machine K-44-2 with type 2 devices (with paper labels on rollers diameter 10 mm). AP and compositions on its basis were tested in the form of pressed (300 MPa) tablets.

Numerical Simulations of Linear Shaped Charge Cutting Using 3D LS-Dyna Code

Piotr Koślik, Zenon Wilk, Waldemar Witkowski

Institute of Industrial Organic Chemistry
Institute of Industrial Organic Chemistry
Institute of Industrial Organic Chemistry

piotr.koslik@ipo.waw.pl, wilk@ipo.waw.pl, witkowski@ipo.waw.pl

Keywords: numerical simulation; LS -DYNA; linear shaped charge.

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

Linear Shaped Charge (LSC) uses high-velocity explosive energy to accelerate a v-shaped liner material (usually copper) into a high-velocity jet that can penetrate and cut the steel. In LSC the initiation is at the end of the charge and after some run up distance the detonations travels down the charge as a vertical plane. Fast dynamics explosive cutting using linear shaped charges numerically simulated by using ALE method 3D LS-Dyna code are presented. Explosive detonation, liner collapse, jet formation and target cutting is analysed in the simulation. The influence of high explosive, liner and target material parameters were studied.

Features of thermal decomposition of nitrate of ammonium in open systems

Igor Kovalenko, Olexandr Kuprin

Ukrainian state university of chemical technology

arragorn@rambler.ru

Keywords: nitrates; thermal decomposition; catalysis; chlorides.

eatures and laws of thermal decomposition of nitrate of ammonium in open system are considered. Catalytic influence of nitrates of sodium and calcium on thermal behaviour of nitrate of ammonium is investigated. Features of catalytic influence of inorganic chlorides on thermal behaviour of saltpetre and systems of nitrate of ammonium / a combustible component are considered.

Design-experiment investigation of mixtures on base of nitrate ammonium, carbamide and biuret

Georgii Kozak, Alexander Starshinov, Olga Litovka, Svetlana Kazakova

Mendelejev University of Chemical Technology

kozakgd@rambler.ru

Keywords: ammonium nitrate; carbamide; biuret; detonation velocity; porous charges.

Porous charges on base of mixtures of nitrate ammonium, carbamide, biuret and aluminium were investigated in this work. Physical and chemical properties of biuret and carbamide were studied by means of differential scanning calorimetry method. Characteristics of fusion of mixtures ammonium nitrate/biuret were studied. At making of charges part of carbamide was replaced with biuret for improvement of detonation characteristics of early studied mixtures. Received mixtures were investigated by method DSC. It was established, what replacement of carbamide on biuret in mixtures of nitrate ammonium/ carbamide / aluminium gives appreciable advantages. Such structures had good stability to moisture and heating to 100 0C without change of density and deformation. Detonation velocity studied mixtures were measured in the work. Detonation velocity, oxygen balance were calculated for mixtures with various densities by SD code. Experimental data were compared with calculated values. Explanation of received results was given in work.

Influence of the current pulse shape to the measurement of electric detonators firing impulse

Dalibor Kuhinek, Igor Zorić, Vinko Šrklec

University of Zagreb

dkuhinek@rgn.hr

Keywords: firing pulse; current pulse shape.

According to EN 13763-19 standard, determination of electric detonators firing pulse is done by applying current pulse to detonator. Activation or nonactivation of detonator is registered and when a sufficient number of detonators are tested, limits of firing pulse can be statistically calculated. Squaring and integrating measured current gives firing impulse as energy divided by total electrical resistance. When testing detonators, it is necessary to generate firing pulses of different levels which is achieved by varying current pulse duration. According to the standard, current pulse can be obtained by discharging capacitor through resistor (exponential fall) or square pulse. Disadvantage of suggested current pulses is required large bandwidth of current recording device. Disadvantage of square pulse is also the difficulty of pulse generation because no significant overshoot is allowed. The device for recording of current has to measure current better than 1 % error limits, which means that it has to have A/D convertor with sufficient number of bits and appropriate frequency response. An 8 bit A/D convertor will have resolution error of 0,39 %. Total limits of error of the oscilloscope are up to 2 %. Noise of measurement system can have significant influence to the error of current recording device. Noise depends on the bandwidth of the measured signal. Using a current pulse shape with smaller bandwidth it is possible to lower noise contribution and increase the accuracy of current measurement. Possible solutions are linear increase and decrease of current in half time of pulse duration or sine shape of current. Measurement system that generates square and sine shape of current is implemented and measurement on electric detonators is done. Current measurement is done by measuring voltage drop over known resistance. Current is recorded by measurement card with 18 bits A/D convertor, oscilloscope with FIR (finite impulse response) filter (11 bits) and additional channel of oscilloscope without FIR filter (8 bits).

The nitration peculiarity of 6-hydroxy-2-methylpyrimidine-4(3H)-one to 6-hydroxy-2-methyl-5-nitropyrimidine-4(3H)-one

Alexander A. Kushtaev, Nikolaj V. Yudin, Vitol'd L. Zbarsky

Mendelejev University of Chemical Technology

kushtaev@mail.ru

Keywords: FOX-7; 6-hydroxy-2-methylpyrimidine-4(3H)-one; nitration kinetic; nitrogen oxides.

The nitration kinetic of 6-hydroxy-2-methylpyrimidine-4(3H)-one to 6-hydroxy-2-methyl-5-nitropyrimidine-4(3H)-one was studied in sulfuric-nitric acid mixtures. The dependences of rate constants from medium acidity and nitric acid concentration were obtained. The nitrogen oxides influence was discovered on this process. The basicity constant of 6-hydroxy-2-methylpyrimidine-4(3H)-one was calculated).

Energetic Parameters of Dinitramine Salts of High Enthalpy Polynitrous Bases

David Lempert, Gelii Nechiporenko, Svetlana Soglasnova

Institute of Problems of Chemical Physics RAS

lempert@icp.ac.ru

Keywords: salts of dinitramine; propellants.

One of ways in new energetic components searching and synthesis is the creation of molecules with high-enthalpy fragments, containing nitrogen, together with oxidizing groups such as -NO2, -NH-NO2, >NNO2, -C(NO2)3, -C(NO2)2NF2 etc. Earlier it was shown that in the set of nitroderivatives of pentatomic unsaturated N-heterocycles (pyrrol, pyrazole, triazole, tetrazole) the increasing of N-atoms amount in the cycle does not conduce a considerable growth of specific impulse of propellants basing on these oxidizers even if the most acceptable binder are used. Another method to increase nitrogen amount in oxidizer is considerable in the presentation, that is the using of salt-oxidizers containing amino-, hydrazine-, azide group, polynitrous pentatomic and hexatomic N-heterocycles as cation with dinitaramine as anion. Energetic parameters of these salts have been studying. As the most of oxidizers under consideration have low oxygen amount propellant basing on these oxidizers have to use binders (polymer and plasticizer) with high active oxygen content. It was shown that the replacement of aminogroup in guanidine on the azide group increases considerable specific impulse, but the replacement of aminogroup on hydrazine groups is more effective - it's possible to create compositions with Isp 270 s (at Pc:Pa=40:1), but at lower density (1.70-1.75 g/cm3). Aminotetrazole salt of dinitramine has high energetic potential - it is possible to get Isp=266 at density 1.85-1.90. Many of dinitramine salts under investigation have the energetic potential higher than ammonium salt of dinitramine has

Detonation characteristics of gasoline/air mixture in pulse detonation engines

Mu Li, Chuan-Jun Yan

School of Power and Energy, Northwestern Polytechnical University
Institute of Fluid Physics, CAEP

Keywords: gasoline; liquid-fueled detonation; pulse detonation engine.

The current focus in utilizing detonation for air-breathing propulsion has moved from oblique detonation waves to investigations and practical development of propulsion engines operating on propagating detonations in a pulse mode. The concept of pulse detonation engine is attractive for both subsonic and supersonic flight with PDC(pulse detonation chamber) as a main combustor or as an afterburner in propulsion unit. In a PDE, detonation is initiated in a tube and the detonation wave rapidly traverses the PDC resulting in a nearly constant-volume heat addition process that produces a high pressure and provides thrust. The operation PDE at high detonation-initiation frequency(about 100Hz) can produce a near-constant thrust. Most of the Pulse Detonation Engine (PDE) related work to date has focused on gaseous mixtures. However, for many practical applications that are volume and weight-limited, the air-breathing PDE will require the use of a liquid fuel. With liquid fuels, additional issues such as atomization, droplet breakup, partial vaporization and incomplete fuel-air mixing (to name a few) must also be considered, and these mixtures are often hard to initiate especially the gasoline/air and kerosene/air. Gasoline/air mixtures are studied in our research as propellant of air-breathing PDEs. Experiments are carried out in a square detonation chamber under the tests condition: normal temperature and pressure, SMD of liquid gasoline spray 20 30 , equivalence ratio 1.2 1.3, dynamic filling velocity 10m/s. Many phenomena such as flame acceleration, shock initiation, hot spots, detonation initiation and propagation in tubes with/without obstacles are observed. Non-ideal detonation are found in most cases with propagation velocity 1000 1500m/s and wave structures of detonation interacting with different obstacles are distinct to CJ detonation wave(1800m/s) in smooth tubes. Cell structures of these mixtures are also recorded on soot foils.

ESD sensitivity of fine grade powdered DMX – Al mixture

Jiri Majzlik

University of Pardubice

Keywords: Al explosive; ESD; sensitivity; testing.

The experimental work was focused on improvement of the methodology of evaluation of sensitivity of fine grain secondary explosives to the effects of electrostatic discharge at the conditions of a small-scale test apparatus ESZ KTTV. A correlation was observed between the energy of electrostatic charge of test condenser, the symptoms of decomposition of the substance tested, and the Joulean energy released during the oscillation discharge directly in the volume of this substance. The findings described can contribute to improvement of methodology of testing fine grain secondary explosives containing metal powder admixtures.

Momentum Method Blast Wave Test for LWC Emulsion Explosives

Andrzej Maranda, Piotr Koślik, Zenon Wilk, Karolina Cieślicka

Military University of Technology
Institute of Industrial Organic Chemistry
Institute of Industrial Organic Chemistry

amaranda@wat.edu.pl, piotr.koslik@ipo.waw.pl, wilk@ipo.waw.pl

Keywords: LWC emulsion explosive; blast wave.

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

Poster present researches of LWC (Low Water Content)emulsion explosives. Tipically near field blast waves and blast momentum results are presented for different charge configurations. Blast impulse load is diagnostic using momentum method - Held's test.

Novel nitrogen rich salts based on 4,5-dicyano-1,2,3-triazole

Franz A. Martin, Margaret-J. Crawford, Thomas M. Klapötke, Konstantin Karaghiosoff

Ludwig-Maximilian University of Munich

fmach@cup.uni-muenchen.de

Keywords: energetic materials; triazoles; guanidinium salts; X-ray diffraction; detonation parameters; sensitivity.

The synthesis of 4,5-dicyano-1,2,3-triazole has been performed as described by known procedures [1]. Going on from there, several nitrogen rich salts, e.g. ammonium-, guanidinium-, aminoguanidinium-, diaminoguanidinium- and triaminoguanidinium- 4,5-dicyano-1,2,3-triazolate have been synthesized and fully characterized. The characterization included low temperature single crystal X-ray diffraction, IR, Raman and NMR-spectroscopy, mass spectrometry and differential scanning calorimetry. The heats of formation have been calculated by the atomization energy method (CBS-4M). With these and the X-ray densities several detonation parameters such as the explosion energy as well as the detonation pressure and velocity have been computed using the EXPLO5 software. In addition the impact, friction and electrical spark sensitivity of all compounds were explored by the BAM drop hammer, BAM friction tester and the OZM small scale electrical discharge device.

Derivatives of nitrated 1,5-Diaminotetrazole – A new class of energetic materials

Franz A. Martin, Jörg Stierstorfer, Thomas M. Klapötke

Ludwig-Maximilian University of Munich

fmach@cup.uni-muenchen.de

Keywords: energetic materials; tetrazoles; nitration; X-ray diffraction; detonation parameters; sensitivity.

The nitration of 1,5-diaminotetrazole (1) with NO2+BF4- yields 5-amino-1-nitramino-4H-tetrazole (2) in good yields. Several nitrogen-rich salts, e.g., ammonium, hydrazinium guanidinium and 1-aminoguanidinium 5-amino-1-nitraminotetrazolate have been synthesized. All compounds have been characterized comprehensively by low temperature X-ray diffraction, IR, Raman and NMR spectroscopy, mass spectrometry and differential scanning calorimetry. Highly endothermic heats of formation were calculated by the atomization energy method (CBS-4M). With these and the X-ray densities several detonation parameters such as the explosion energy as well as the detonation pressure and velocity have been computed using the EXPLO5 software. In addition the impact, friction and electrical spark sensitivity of all compounds were explored by the BAM drophammer, friction tester and the OZM small scale electrical discharge device. 2 can also be used as a new ligand in transition state metal complexes, which was proofed by the reaction with copper nitrate yielding trans[tetraaqua-bis(5-amino-1-nitraminotetrazolato-N4)-copper(II).

TEX as a Component of Plastic Bonded Explosives

Andrzej Orzechowski, Lucjan Staszewski, Dorota Powała, Andrzej Maranda

Institute of Industrial Organic Chemistry
Military University of Technology

orzechowski@ipo.waw.pl, staszewski@ipo.waw.pl

Keywords: 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diaza-tetracyclo [5,5,05,9,03,11] dodecane; TEX; PBX.

In this paper, the methods of synthesis and crystallization of 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diaza-tetracyclo [5,5,05,9,03,11] dodecane(TEX) are presented. The obtained TEX was applied to a preparation of plastic bonded explosives (PBX). The explosive properties and sensitivity to external stimuli of PBX were tested. The PBX composition and method of obtaining usable form were selected after several experiments. The measurement results of detonation velocity, Gap-test and sensitivity to impact of pressed charges are described.

Solid Nitroglycerine Analoga With Improved Energetic Properties

Alex Penger, Thomas Altenburg, Susanne Scheutzow, Lukas Vejs, Thomas M. Klapötke

Ludwig-Maximilian University of Munich
OZM Energetic Materials Research

pench@cup.lmu.de

Keywords: nitroglycerine; nitramines; crystal structure; performance.

1,3-Dinitramino-2-nitroxypropane (NG-A1) is an energetic compound known for nearly 60 years, but there has not been an attempt to prove its energetic properties with regard to its isolable analogue nitroglycerine. Another new analogues compound, namely 1-nitramino-2,3-dinitroxypropane (NG-A2) was fully characterized. The physical properties of these compounds can be derived from their arrangement in the solid state. A low melting point of NG-A2 makes this compound suitable for meltcast applications. Energetic properties were measured with bomb calorimetry and proved with computational methods and experimental determined detonation velocity. Both compounds have performances and sensitivities comparable to RDX.

Some Properties of PBX Contain FOX-7

Dorota Powała, Andrzej Orzechowski, Andrzej Papliński, Andrzej Maranda

Institute of Industrial Organic Chemistry
Military University of Technology

powala@ipo.waw.pl, orzechowski@ipo.waw.pl

Keywords: PBX; FOX-7; explosives.

In this paper, the methods of synthesis and crystallization of 1,1-diamino-2,2-dinitroethylene(FOX-7) are presented. The obtained FOX-7 was applied to a preparation of plastic bonded explosives (PBX). The explosive properties and sensitivity to external stimuli of PBX were tested. The PBX composition and method of obtaining usable form were selected after several experiments. The measurement results of, Gap-test and sensitivity to impact, detonation velocity of pressed charges are described.

Study regarding effectiveness of stabilizer revival process on old artillery propellants. Part 2

Traian Rotariu, Doru Adrian Goga, Sorin Razvan Esanu, Tudor Viorel Tiganescu, Marius Valeriu Cirmaci

Military Technical Academy

traianrotariu@yahoo.com

Keywords: nitrocellulose; propellants; simple base; diphenylamine; stabilizer.

The paper is a continuation work of that presented in NTREM 2008. It deals with further experimental investigations performed in order to evaluate safety and performance characteristics of some old simple base propellants for large calibre ammunition, after a "revival" process consisting in supplementary diphenylamine (DPA) addition. Revived propellants were tested comparative to new and old propellants of similar composition and geometry.

Synthesis of energetic compounds from 5-azido-2,2-dimethyl-5-nitro-1,3-dioxane

Gennady Rudakov

Mendelejev University of Chemical Technology

rudakov@rctu.ru

Keywords: 1,3-dipolar cycloaddition; 1,2,3-triazoles; nitroazides; nitroesters.

The synthesis of 1,2,3-triazoles via 1,3-dipolar cycloaddition of 5-azido-2,2-dimethyl-5-nitro-1,3-dioxane to propargyl alcohol and 2-butyne-1,4-diol is reported. New azidomethyl- and nitroxymethyl-1,2,3-triazole derivatives have been synthesized from products of these addition. The new 1,2,3-triazoles have been identified by means of IR, 1H, 13C NMR spectral and elemental analyses. Thermal behavior of new compounds has been studied by means of TGA/DTA analysis.

Precipitated RDX and TAGN particles for use in propellants

Radovan Skácel, Jan Zigmund, Pavel Mareček, Pavel Prchal, Martin Karnet, Jan Skládal

Explosia a.s.

radovan.skacel@explosia.cz

Keywords: TAGN; triaminoguanidine nitrate; RDX; cyclonite; propellants; precipitation.

In search of a method to replace expensive and time-consuming milling process when preparing fine TAGN and RDX crystals of appropriate surface area the method of precipitation was tested. Samples of precipitated TAGN and RDX particles were experimentally prepared using various solvents and precipitators under various conditions, in some cases under presence of suitable polymere matrix. In certain cases a diameter of the crystals obtained was below required 5 mm. This size crystals were then tested as a component of ball powders and green propellants.

Bistetrazolyltetrazenes as energetic, nitrogen rich compounds

Stefan Sproll, Thomas M. Klapötke

Ludwig-Maximilian University of Munich

sspch@cup.uni-muenchen.de

Keywords: bistetrazolyltetrazene; tetrazene; energetic; nitrogen rich.

Several bistetrazolyltetrazenes were synthesized as nitrogen rich, energetic compounds in high yields using common procedures. All compounds were characterized by vibrational spectroscopy (IR, Raman), mass spectrometry and multinuclear NMR spectroscopy. The crystal structures of the compounds were determined using single crystal X-ray diffraction. In addition the thermal behavior of the tetrazenes was monitored using differential scanning calorimetry. The energetic properties were investigated by bomb calorimetric measurements and calculations using the EXPLO5 software.

Explosive formation and spreading of water-spray cloud – Experimental development and model analyses

Krzysztof Stefański, Damian Lewandowski, Roman Dygdała, Grzegorz Śmigielski, Michał Kaczorowski, Maria Ingwer Żabowska, Andrzej Papliński

Szkoła Wyższa im. Pawła Włodkowica
Wyższa Szkoła Gospodarki
Mikołaj Kopernik University
Military University of Technology

stefan@fizyka.umk.pl, damian_lew@wp.pl, romdy1@onet.pl, gsmigielski@byd.pl

Keywords: explosion; water aerosol production; shock wave parameters.

The paper presents results of experimental investigations and model analysis con-cerning of expansion of explosively produced water-spray cloud. The regular shape of water-spray cloud produced of by a charge placed in a bag filled with water is attained. Effective dispersion of bags containing of 600 up to 1500 litres of water is attained. The rise and deceleration of external zone of water-spray cloud is de-scribed analytically. The parameters of pressure field evolving around the explo-sively formed spray cloud were registered.

Influence of structure on the thermal decomposition rate of formals of polynitroalcohols in liquid phase

Rudolf S. Stepanov, Ludmila A. Kruglyakova, Alexander M. Astachov

Siberian State Technological University

Keywords: formals of polynitroalcohols; kinetics; thermal decomposition.

The thermal decomposition of formals of polynitroalcohols in liquid phase proceeds by the homolytic mechanism with primary break of C-NO2 bond. Nitrogen oxide oxidizes intermediate decomposition products and original compound. The volume of substituent at geminal dinitrogroup and its conjugation with reaction center has a strong influence on the constant of decomposition rate. The correlation dependence is found between decomposition rate constant and steric constant of substituent Es.

A Green Replacement of Lead Azide: Calcium 5-Nitriminotetrazolate

Jörg Stierstorfer, Thomas M. Klapötke

Ludwig-Maximilian University of Munich

jstch@cup.uni-muenchen.de

Keywords: energetic materials; primary explosives; tetrazoles; X-ray; sensitivity.

In this work we present our most powerful and qualified replacement of lead azide in priming charges, calcium 5-nitriminotetrazolate (1). This compound can be prepared by a facile synthetic route, also in larger scales. 1 shows great performance in initiation experiments of hexanitrostilbene on the one hand side and an astonishing thermal stability as well as long term stability on the other hand side. Next to the detailed synthetic procedure and dehydration process, a comprehensive characterization including X-ray diffraction, vibrational spectroscopy, NMR spectroscopy and differential scanning calorimetry is described. The heat of formation has been calculated by the atomization energy method. Lastly, the sensitivities of 1 were investigated by the BAM drophammer and fiction tester as well as a small scale electrical discharge device.

Study of mechanical properties of rocket DB propellant during natural ageing

Muhamed Sućeska, Sanko Bakija, Janoš Kodvanj, Sanja Matečić Mušanić, Ivona Fiamengo, Ante Bakić

Brodarski institute-Marine Research & Advanced Technologies
Ministry of Defence of the Republic of Croatia
Faculty of Mechanical Engineering
and Naval Architecture

suceska@hrbi.hr

Keywords: mechanical properties; rocket propellants; natural ageing; dynamic mechanical analysis; tensile test.

Various chemical reactions and physical processes (such as stabilizer consumption, migration and evaporation of NG, decomposition of NG and NC, etc.) take place in rocket propellants grains during the time, even under ambient storage conditions. The overall effect of these reactions and processes are the change of physical, chemical, thermal, ballistic and mechanical properties of rocket propellants with storage time, i.e. the reduction of the propellants performances and safe service life. The aim of this work was to evaluate mechanical changes of rocket propellant – sustainer, as a part of in-service ATGM system, induced by "natural" ageing after many years of storages. The results of the mechanical properties testing of double base rocket propellants in some selected antitank guided missiles (ATG), stored under ambient conditions up to 35 years, are presented in this paper. The mechanical properties are tested using dynamic mechanical analysis (DMA), uniaxial tensile and compression tests, and notch toughness test. It was found out that the trend of changes of the mechanical properties during the storage time is evident, although in some cases the results of the tests are rather scattered (as a consequence of measuring uncertainty) and changes of some mechanical properties are not too pronounced. For example, after 15 years of storage at ambient conditions the glass transition temperature increases for about 5 °C, tan in the glass transition region decreases for about 5%, storage and loos modulus at 25 °C increase for about 15%, Young modulus at 23 °C increases up to 30%, notch toughness at -30 °C decreases up to 15 %, etc. Other mechanical characteristics showed small but not significant trend of changes. Along with those tests, the stabiliser content and proving ground test were also done.

The dependence of composition gun shot residues on the gun barrel lenght

Václav Svachouček, Petra Svachoučková, Ladislav Velehradský, Karel Ventura

Svachouček
Defence Standardization, Codification and Government Quality Asssurance Authority
Explosia a.s.
University of Pardubice

Keywords: gun shot residues; ammunition; analysis.

Currently, the study of gun shot residues constitutes a wide and a very interesting problem as from the shooter´s view so as from the design enginneers´ view and furthermore possibilities, which influence the conditions of the process of products formation. Currently, one direction of the investigation of gun shot residues proceeds the study of morfology and thereby even possibilities of improvement of firm particles and further physical conditions, which influence for instance their stability in the surveyed environment or scatter particles. This problem is investigated by research police institutes above all. The detection of the shot place from the specific cartridge of a concrete weapon is the object of their investigation. The lay formation of gaseous gun shot residues and their possible toxicity is interesting from the gunner´s view. We have been dealing with this problem for 5 years. This lecture is intented on the problem of the dependence of composition of gaseous gun shot residues on the gun barrel lenght.

Voltammetric redox behavior of high energy aromatic and N-heterocyclic nitrocompounds

Jonas Šarlauskas, Kastis Krikštopaitis, Kęstutis Sekmokas, Narimantas Čenas

Institute of Biochemistry

hidrazon@bchi.lt

Keywords: nitrobenzenes; nitroheterocycles; explosives; cyclic voltammetry; reduction potential.

The environment contamination by explosive nitroaromatic and nitroheterocyclic compounds is an important problem. The toxic action and biodegradation of the above compounds is mostly related to their 1e-/2e-(4e-) flavoenzyme-catalyzed re-duction. In order to understand their bioreduction mechanisms and enzyme sub-strate specificity, as well as to foresee the pathways of their biodegradation, one has to characterize their electron-accepting properties. In this work, we performed cyclic voltammetry studies (pH 7.0, aqueous medium) of a number of nitrobenzenes, nitroderivatives of 1,2,4-triazole, tetrazole, benzimidazole, and benzofuroxan. Their reduction peak potentials ranged from -73 to - 978 mV vs. Ag/AgCl, being dependent on the electron-accepting properties of the ring substituents. Typically, the reduction peak current was proportional to the square root of the potential scan rate, which is consistent with the diffusion-controlled electrochemical process.

Decomposition kinetics of urea nitrate

Jakub Šelešovský, Robert Matyáš

University of Pardubice

Keywords: urea nitrate; decomposition; kinetics; thermal analysis.

The decomposition kinetics of urea nitrate (UrN) was determined by several meth-ods of thermal analysis. Isothermal and nonisothermal thermogravimetry and iso-thermal vacuum stability test were used. The measured data were processed using the non-parametric kinetics method. The Arrhenius parameters differ in depend-ence on the measurement technique used. The influence of measurement condition, especially the pressure and the atmosphere on the obtained kinetic parameters is discussed.

Transformation of aluminum at explosion of its mixtures with benzoyl peroxide.

Alexander Tsvigunov, Ilya Zhukov, Georgii Kozak, Vlada Raikova

Mendelejev University of Chemical Technology

Keywords: peroxides; benzoyl peroxide; aluminium; aluminium hydride; aluminium oxide; HMX; synthesis; explosion at impact.

Mixtures of benzoyl peroxide with different forms of aluminium (aluminium powder, aluminium hydride), benzoyl peroxide with ammonium nitrate and different forms of aluminium, benzoyl peroxide with HMX and aluminium hydride were studied. Mixtures of HMX with aluminium hydride have been studied for comparison. X-ray diffraction analyses of explosion products have been carried out. Difference between organic peroxides and typical energetic materials was shown in this work. And 2 new forms of aluminium oxide have been synthesized at explosion of mixture HMX with aluminium hydride.

A theoretical Study of 1.1-dinitropropane decomposition

Roman Tsyshevsky

Kazan State Technological University

tsyshevskyrv@rambler.ru

Keywords: 1,1-dinitropropane; B3LYP.

Some properties of decomposition pathways of 1,1-dinitropropane were studied computationally at the B3LYP level of theory with 6-31G(d) basis set. All calculations were performed with the program Gaussian 98. Several possible channels for the decomposition of 1,1-dinitropropane and its radical cation: dissociation through direct breaking of the C-N bond, producing two radicals, elimination of HONO, nitro-nitrite rearrangement, and finally a mechanism of hydrogen transfer and isomerisation to aci-form were studied.

Computational investigation of nitroglycol (EGDN), ethylenedinitramine (EDNA) and their sulfur analogs (thionitrates)

Lemi Türker, Taner Atalar, Hamza Turhan

Middle East Tecnical University

lturker@metu.edu.tr

Keywords: nitroglycol ; EGDN; possible energetic materials; computational study.

Some energetic materials, ethane 1,2-dyl dinitrate (EGDN) (1), N,N'-(ethane-1,2-diyl)dinitramide (EDNA) (2), and some possibly energetic materials, S,S'-ethane-1,2-diyl dinitrothioate (3), S-2-(nitroamino)ethyl nitrothioate (4), 2-(nitrothio)ethyl nitrate (5), 2-(nitroamino)ethyl nitrate (NENA) (6) , have been considered, their univalent charged forms (-1, +1) are also investigated quantum chemically, using density functional theory (DFT-UB3LY/6-311+G (d,p)). Various geometrical parameters, energies have been obtained and discussed. In order to compare the termal stabilities of them, homolytic bond dissociation energies (C-C, C-N, C-O, C-S, N-NO2, O-NO2 and S-NO2) are computed by using DFT. Also, detonation performances were evaluated within the limitations the Kamlet-Jacobs equations, based on the quantum chemically calculated densities and heat of formation values.

Detonation parameters of watergel aluminum-containing explosives

Anna Veprikova, Vladimir Annikov, Vladimir Trunin, Alex Apolenis, Vlada Raikova

Mendelejev University of Chemical Technology

a.veprikova@mail.ru

Keywords: watergel explosives; aluminium; detonation; electromagnetic technique.

Water-impregnated aluminum-containing compositions (WE) are used as commercial explosives for rock blasting, seismic investigations and other purposes. They are safe and incombustible explosive materials characterized by very low levels of mechanical and heat sensitivity. A variety WE containing solutions based on ammonium, sodium and calcium nitrates were explored by Prof. B.N. Kondrikov and Dr. V.E. Annikov at Russian Mendeleev University of Chemical Technology. On the basis of this work, a series of compositions water-impregnated, commercial explosives were developed and some of them successfully introduced into industry. For series WE, mostly of the gelled type, containing different quantities of finely dispersed aluminum the dependencies of detonation velocity on density and on the charge diameter, failure diameter of detonation as well as critical density corresponding to the loss of detonation ability of the charge were measured. The main objective of this work is study of detonation parameters (particle velocity u, detonation velocity D and detonation pressure P) for gelled WE containing nitrates of ammonia and sodium and aluminum powders. The mass fractions of water and ammonium and sodium nitrates were chosen as 2.5:1.5:1, correspondingly. The weight percent of aluminum in the formulations ranged from about 5 to 50%. For gelatinization of mixtures the polyacrylamide (1.2%) was added. Detonation experiments were carried out in paper casing charge with diameter 32 and 20 mm and about 40 mm long. Measurements of profiles of particle velocity vs. time, u(t), and detonation velocity, D, carried out by means of electromagnetic technique. Values of pressures at detonation wave were calculated and the profiles, P(t), were determined too. Influence of content of various aluminum powders on detonation parameters was examined.

Application of optic inspection in solid propellants strength experiments

Tomasz Wolszakiewicz, Tomasz Gawor

Institute of Industrial Organic Chemistry

wolszakiewicz@ipo.waw.pl

Keywords: solid propellant; strength experiments.

Application of optic inspection allows for video recording of cracking process in solid rocket propellant specimens during static tension tests and under fatigue loads. Digital analysis of recorded cracking process is based on digital correlation of images. Obtained test results of cracking parameters allow for their connection with specimen load parameters.

Viscoplastic model for solid propellants

Robert Zalewski, Tomasz Wolszakiewicz

Institute of Machines Design Fundamentals Warsaw University of Technology
Institute of Industrial Organic Chemistry

robertzalewski@wp.pl, os65@wp.pl

Keywords: propellants; experimental studies; modeling; constitutive law; numerical simulation.

In order to improve the operational safety of special objects, working on the basis of solid propellants, and to increase their durability and resistance on extreme working conditions, it is essential to understand the complex physical phenomena observed in energetic materials. Problematical extreme operational conditions are related to a particularly aggressive working environment, a frictional wear of solid propellants and a degradation of mechanical properties, caused by temperature gradients. Typical experimental methods applied in solid propellants are analogical (from the mechanical point of view) to experimental methods of solid materials or plastics. Generally, they are restricted to the most popular uniaxial experiments, mainly due to economical limitations. The tests are realized on standard tensile testing machines. Typical mechanical parameters, examined during laboratory tests, are Young modulus, Poisson ratio, tensile strength or yield limit. To provide a suitable constitutive model for solid propellants, a lot of fundamental experiments have to be carried out. It is particularly interesting, that general standards for conducting basic strength properties experimental tests have not yet been fully elaborated for this class of materials. Such problems as quasi-static strain range for solid propellants or shape and dimensions of simple testing specimen are still not normalized. Also, the available data concerning the basic rheological properties of solid rocket fuels is insufficient. Though, this paper is a preliminary investigation devoted to modeling of nonlinear properties of solid propellants. The paper discusses experimental results obtained for a selected group of solid propellants. The viscoplastic constitutive model of Chaboche is proposed to model nonlinear properties of the studied material. An effective analytical method of model parameters identification is applied. The results of numerical simulations are in very good agreement with experimental data.

Eutectic Compound of Perchloric Amine Salt

Shunguan Zhu

Nanjing University of Science and Technology

zhusg@mail.njust.edu.cn

Keywords: perchloric amine salt; primary explosives; eutectic compound.

This paper describes the studies carried out on the eutectic compound of amine perchlorate. This eutectic compound (SY) reported in this paper is the combination of triethylene diamine (TEDA) perchlorate (SE) and ethylene diamine (EDA) perchlorate (YE). The composition ratio of the SE and YE is 1:1. The eutectic compound produced from the SE and SY has been evaluated for its initiating ability. The eutectic compound (SY) obtained was characterized by FTIR and 1H NMR spectroscopy. The physicochemical properties such as density, solubility in various solvents, hygrscopicity have been studied and reported in this paper. The eutectic compound obtained has also been studied for its thermolysis behavior using hyphenated differential scanning calorimetry (DSC)- thermogravimetry (TG). The explosive properties such as ignition temperature (explosion point), impact and friction sensitivity, and velocity of detonation, brisance and initiating power of the compound have been studied The initiating power of the eutectic compound (SY) to the RDX increases nearly four times than SE or YE. The experimentally determined velocity of detonation (VOD) was found 7240m/s under the charge density of 1.65g/cm3. Its brisance is 20.0 mm, which is 1.21 times of TNT. The expanded volume in lead block is 398 ml, which is 1.37 times of TNT.

Keyword Index

Author Index

The End