Abstracts of the 13th Seminar on

New Trends in Research of Energetic Materials

Pardubice, April 21–23, 2010

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

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

Abstracts of the 13th Seminar on

New Trends in Research of Energetic Materials

Held at the University of Pardubice and devoted to
ninety years
of education in the field of Science & Technology of Explosives
in the former Czechoslovakia

Pardubice, Czech Republic
April 21–23, 2010

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

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Part 2

Posters

90 Years of Teaching of Chemistry and Technology of Explosives in Bohemia

This year is the 90th anniversary of start of education in the field of chemistry and technology of explosives in the then Czechoslovak Republic. In 1920, these scientific-pedagogical activities were started at the Institute of Chemical-Technological Engineering (the present Institute of Chemical Technology Prague – VŠCHT Praha) under the guidance of Dr. Cyril Krauz. In the same year, the factory Explosia, manufacturing explosives, was established at Pardubice. These two events significantly affected the development in the area of energetic materials in Czechoslovakia, which was a young republic formed in 1918 after the break-up of Austro-Hungarian Monarchy. The said development together with the high standard of the then Czech machinery industry resulted in the fact that before the Second World War Czechoslovakia became a significant producer and exporter of weapons, ammunition and explosives with corresponding scientific-research and engineering background.

The education was shut down in the period of the Second World War, when universities and colleges on the occupied Czech territory were closed (1939–1945). After post-war restoration of scientific-pedagogical activities at these colleges, a sub-branch called "Technology of Special Production" was established at the Department of Organic Technology VŠCHT Prague in the academic year 1952/1953. Dr. Ing. Josef Seifert was appointed as its head, and he, using his personal contacts at Pardubice, in the same academic year prepared establishing of Department of Technology of Special Production at the Institute of Chemical Technology Pardubice (VŠCHT Pardubice). This Institute was established at Pardubice in 1950; hence it is going to celebrate the 60th anniversary of its existence, now as Faculty of Chemical Technology, University of Pardubice.

September 1953 can be considered as official time point of creation of the Department of Special Production at VŠCHT Pardubice, the predecessor of the present Institute of Energetic Materials (IEM). The workplaces of IEM were and have remained the only ones of this sort on the territory of former Czechoslovakia. So far, 326 students have graduated from IEM at the MS (engineer) level, more than 400 students have got through two courses of extramural studies (technological course and course of blasting), and 67 students have graduated at the PhD level. These graduates include also foreign citizens (from Hungary, Afghanistan, Yugoslavia and Egypt).

In the past, IEM significantly participated in developing industrial explosives for a Slovak manufacturer – Istrochem Bratislava, dealt with practical problems of occupational safety in the factories endangered by explosion risks within Czechoslovak industry particularly in the area of underground coal mining, and with problems connected with developing of some special explosives and initiators. In the period following the political transformation of November 1989, IEM has been continuing its cooperation with Slovak manufacturers in the field of development of high explosives. At present, IEM is pursuing activities in the area of development of environmentally friendly primary explosives and initiators, dealing with problems of safety engineering in the area of explosion of gaseous and disperse systems and in the field of risk analysis. Apart from pedagogical activities directed to full-time students at MS, PhD and (in part) BSc levels, IEM extensively organizes extramural courses both in theory & technology of explosives and in blasting for experts from practice. The pedagogical activities also include participation in dealing with European projects concerning development of educational programs for education of all those working in the branch of explosives (EUExnet) and separately also education of shot firers in the framework of the ESSEEM program.

Other significant activities of IEM involve organization of international seminars "New Trends in Research of Energetic Materials" (NTREM). The original stimulus for starting the NTREM seminars was an attempt at teaching young research workers how to present their results in front of scientific audience. Now, the

meetings are first of all meant for undergraduates, PhD students, young workers in scientific research and university teachers in the field of energetic materials (research, development, production, handling, environmental issues, testing, application) and the therewith connected safety engineering. With regard to the fact that the participants are young people, no fees were required at the Seminar. However, the price trends existing in the Czech Republic over the past two years led to a change: although the practice of not asking the participants to pay any fee has been continuing, nevertheless a voluntary donation of €100 is appreciated.

Realization of our seminars would never be possible without the generous support from many institutions. The 13th NTREM seminar has been financially supported by:

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The efficient help obtained from all these institutions in ensuring smooth and successful course of the meeting 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.

And traditionally, what should I add on the occasion of this 13th 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, March 10, 2010

Svatopluk Zeman

Ageing study of a polymer bonded explosive

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TNO Defence, Security and Safety

Keywords: ageing; PBX.

In this study the PBX KS-32 was investigated to obtain a better understanding of the relationship between the ageing by temperature and the physical or chemical changes that affect the hazard properties of the composition, identifying the critical degradation mechanisms, examining the effects of inhomogenity and looking at the changes in the mechanical properties.

To obtain all the necessary information, various techniques have been used for analyzing the aged and un-aged materials. For the mechanical properties Dynamic Mechanical Analysis (DMA) is used, for the chemical properties High Performance Liquid Chromatography (HPLC) and Attenuated Total Reflection Fourier Transform Infrared (ATR-FTIR) spectroscopy. The physical properties of the un-aged and aged materials were obtained from the friction apparatus, for impact the Fallhammer system and friability tests to obtain information about the insensitive munitions (IM) property. Kinetics, decomposition and glass-transition temperature were determined with the thermo gravimetric analysis; the degradation gasses with mass spectrometry and infrared spectroscopy. The glass-transition temperatures of the sample were also obtained from DMA.

The main tasks in solid composite propellants performances improving

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Russian Academy of Science

Keywords: solid composite propellants; specific impulse; density; combustion temperature; formation enthalpy.

The lecture considers different kinds of solid composite propellant (SCP). All ways to increase energetic potential of SCP are considered, such as heat release increasing (the use of metals as energetic compounds, the use of compounds with an active fluorine, formation enthalpy of compounds increasing) as well as the increasing of light gases (mainly hydrogen) fraction in the combustion products (the use of onium salts as oxidizers, hydrazinium groups introducing, the use of hydrides of aluminum or beryllium, hydrides of boron and BHN-compounds). Each of forecited ways has its own pro et contra, and naturally definite limits. The investigation is aimed to attract an especial attention to discuss such problems, because nowadays the energetic parameters of SCP using chemical energy is approaching to the definite limit afore which all other properties (thermal stability, impact and friction sensitivity, combustion temperature, combustion low, cost etc) degrade drastically. Influence of oxidizer, binder, metal nature on the energetic parameters of the SCP formulations is considered in the lecture. Different kinds of oxidizer (perchlorates of ammonium, hydroxylammonium, and hydrazinium; ammonium salt of dinitramine; other saltlike and molecular oxidizers) are under consideration. It was shown that the effectiveness of metal introduction into the formulation depends strongly on the total formation enthalpy of the formulation (mainly, on the oxidizer's enthalpy). It is not effective to add aluminum into the formulation basing on high-enthalpy oxidizer (with Δ^{o}Hf value 200-400 kcal/kg and higher) – the specific impulse does not rise practically any more. The main principles of SCP formulation creation with optimal characteristics in the context of their concrete purpose are discussed, e.g. for rockets with considerably low ratio propellant volume/empty construction mass (V/M lower than 1 Litr/kg or so) the ballistic effectiveness may be increased with the replacement of aluminum for high-dense zirconium or its hydride. Problems of creation of special SCP kinds with lower environment pollution (such as HCl) are considered too as well as specific formulations for application at the far space, e.g. for Mars exploration. Abilities of further improvement of energy and other properties of SCP are under consideration in the presentation.

Diagnostic techniques in deflagration and detonation studies

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Keywords: high-speed; quantitative.

This paper will review a number of experimental, high-speed techniques which have been used to explore, in a time-resolved fashion, the processes occurring within energetic materials. A wide range of processes will be covered; hot-spot formation, ignition thresholds, deflagration, sensitivity and finally the detonation process. This is a wide field and so, the focus will be on small-scale experiments and quantitative studies. It is important that such studies are linked into predictive models and also in the design process. Examples taken from this group's research will include drop-weight, Hopkinson Bar and Plate Impact studies. Studies made with inert materials will be mentioned in order to differentiate between reactive response and purely mechanical behaviour.

Preparation and properties of novel fluorescence alkynyl compounds for explosive detection

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Keywords: fluorescence alkynyl compounds; quantum chemistry; explosives detection; fluorescence quenching; sensing materials.

9-hydroxy-9-acetenylanthrone was synthesized via nucleophilic addition reaction and the elimination of trimethylsilyl under base catalysis. Its structure has been confirmed by IR ,1H NMR and LC-MS, what is more, its melting point, crystallization, Uv spectra and fluorescence spectra were also obtained. Its molecular structure, the distribution of charge and stationary potential were calculated by quantum chemistry at B3LYP/6-31g(d,p) level. The emission spectra of 9-hydroxy-9-acetenylanthrone has been investigated in chroloform and methanol. The maximum excitation wavelength and emission wavelength were estimated under 1.1 mmol/L 9-hydroxy-9-acetenylanthrone in chloroform, i.e. 376nm and 443nm respectively. The fluorescence quenching of TNT to 9-hydroxy-9-acetenylanthrone has been determined. The results showed that TNT could quench the fluorescence of 9-hydroxy-9-acetenylanthrone obviously. 9-hydroxy-9-acetenylanthrone would be used as sensing material for detecting explosives.

Detonation properties of mixtures of ammonium nitrate based fertilizers and aluminium

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Keywords: ammonium nitrate based fertilizers; detonation properties; illicit use of explosives.

Detonation velocity and Guerney's energy of mixtures of ammonium nitrate based fertilizers and aluminium have been determined. The fertilizers were ammonium nitrate or its mixtures with dolomite (CAN). Results show that even from mixtures of CAN and aluminium strong explosive may be prepared.

Ageing of HTPB/AP/Al rocket propellant formulations investigated by dynamic mechanical analysis and sol-gel analysis

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Keywords: HTPB propellants; ageing; DMA; sol-gel analysis; GPC analysis; loss factor evaluation; molecular mobility changes.

Solid rocket propellants (SRP) based on HTPB / AP / Al (binder hydroxyl terminated polybutadiene / ammonium perchlorate / aluminium powder) are at time the choice to achieve high performance with high specific impulses. In general, such SRP are relatively ageing resistant compared to NC-based double base propellants. But also such propellants change their properties with time. Ageing mechanisms are: after-curing, chain scission by mechanical overload during temperature cycling, oxidative hardening together with loss in strain capability, oxidative chain scissioning, dewetting between particulate fillers (especially AP) and binder matrix.

In this work DMA (Dynamic Mechanical Analysis) in torsion mode and Sol-Gel-Analysis (SGA) have been employed together with SEM (Scanning Electron Microscopy) and GPC (Gel Permeation Chromatography) to elucidate the ageing behaviour of four HTPB-based SRP, whereby the particle size of aluminium powder was changed also. The accelerated ageing range was between 60°C and 90°C with ageing times adjusted to a thermal equivalent load of 15 years at 25°C.

The investigations with DMA revealed distinct changes in the shape of the loss factor curve. The loss fac-tor gives the part of applied deformation energy, which is consumed by the sample. The other part is transported through the sample to the response detector. Detailed analysis of the shape of the loss fac-tor showed that three parts of molecular rearrangement types can be identified during the total transi-tion of the material from energy-elastic to the entropy-elastic state. For this a special treatment and modelling of the loss factor curve is necessary, which was developed. One part of the curve is the main binder rearrangement, which is nearly not changed during ageing, thanks to the action of the used an-tioxidant. Another main part is assigned to restricted movements around the particulate fillers, especially AP particles. This part decreases with ageing. A third part is situated between the main chain binder part and this restricted part and it increases with ageing. This phenomenon is interpreted by a change in binder–filler bonding. SEM analysis revealed a dewetting of the particles and this is consistent with the DMA results.

The results of SGA showed a complex change in soluble or extractable polymeric binder part. Both cross-linking and to some part also chain scissioning occur, which could be recognized by the changes of the molar mass distribution functions of the extractable binder part.

Four syntheses of 4-amino-3,5-dinitropyrazole

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Keywords: energetic materials; 4-amino-3,5-dinitropyrazole; synthesis; pilot plant scale.

In this paper, syntheses of 4-amino-3,5-dinitropyrazole from four different starting materials are described. The starting materials are 4-nitropyrazole, 4-nitro-3,5-dimethyl¬pyrazole, 3,5-dinitropyrazole and 4-chloropyrazole, respectively. They are compared in terms of yield, number of steps, price of starting materials and suitability for scale-up into pilot scale production. The overall yield, calculated from commercially available starting materials, ranged from 21 % in the case of synthesis via 3,5-dinitropyrazole up to 46 % for the on starting from 4-chloropyrazole. The cheapest starting material was 3,5-dimethylaminopyrazole and the most expensive 4-chloropyrazole. With numerous factors taken into account, the latter was chosen for a pilot scale study and the product could be produced in batches of 200g.

Detonation Characteristics of Bicyclo-HMX and HNIW with Two Different Binders

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Keywords: explosives; detonation; C4 matrix; BCHMX; HMX; HNIW; RDX; stability; viton.

Bicyclo-HMX (cis-1,3,4,6-tetranitro-octahydroimidazo-[4,5-d]imidazole or BCHMX) was studied as a plastic explosive bonded by the C4 matrix and by Viton A. Also a series of nitramines namely RDX (1,3,5-trinitro-1,3,5-triazinane), HMX (1,3,5,7-tetranitro-1,3,5,7-tetrazocane) and HNIW (ε-2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane, ε-CL-20) were studied with the same types of binders. The detonation velocity, D, of all prepared mixtures was measured. Their thermal stability was determined using differential thermal analysis (DTA) and approximate relationships between the peaks of exothermic decomposition and their D values were found. The detonation parameters were also calculated by means of Kamlet & Jacobs method for all the mixtures in addition to CHEETAH and EXPLO5 codes for the mixtures based on the C4 matrix. From the measured D values and the calculated detonation parameters, it is obvious that the detonation parameters of BCHMX-C4 are very close to HMX-C4 and better than those of RDX-C4. The D values of pressed BCHMX-Viton A is lower than that of HMX-Viton A, and also higher than in case of RDX-Viton A. As expected, the pressed HNIW-Viton A mixture has the highest detonation parameters of all of the prepared mixtures.

Study of over-compressed regimes of detonation of condensed HE with use of laser doppler velocimeter

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Keywords: over-compressed detonation; condensed HE; two-stage loading; Fabry-Perot method.

Over-compressed regimes of detonation of condensed HE were investigated. Over-compression magnitude was varied within 1.1 . . . 2.4 times. Various types of particle velocity profiles of over-compressed wave were recorded. Smooth declining profiles of DW were recorded at weak over-compression ($\approx$ 10 %). When pressure in over-compressed wave is close to the point of crossing of the initial HE adiabat and EP isentrope (over-compression is 30-35%), profiles with constant value of particle velocity were recorded. At the maximum over-compression of 2.4 times in plasticized PETN, smooth growth of wave parameters in the profiles was recorded in the pressure range of 49-58 GPa for 90 ns. In our opinion, the reason is that high pressures compress explosion products and decelerate growth of the chemical reaction.

Energetic materials based on 1-amino-3-nitroguanidine

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Keywords: 1-amino-3-nitroguanidine; energetic materials; crystal structure; detonation parameters; sensitivity.

1-Amino-3-nitroguanidine (1) was synthesized by hydrazinolysis of nitroguanidine. Due to its basicity, it can easily be protonated by energetic compounds bearing an acidic proton. The 5 nitrimino-4H-tetrazolate (2), 1-methyl-5-nitriminotetrazolate (3) and 2-methyl-5-nitriminotetrazolate (4) salts were synthesized. 5-Nitrimino-1,4H-tetrazole was obtained by reacting 5-amino-1H-tetrazole with 100% HNO¬3. 1-Methyl-5-nitriminotetrazole and 2 methyl-5-nitriminotetrazole were obtained by methylation of sodium 5-aminotetrazolate with dimethyl sulfate, followed by the nitration using also 100% HNO3. Furthermore, the dinitramide (5) and perchlorate (6) salts of 1-amino-3-nitroguanidine were synthesized by protonation of 1 with 60% perchloric acid and reaction of potassium dinitramide with the perchlorate salt 6, respectively. All compounds were fully characterized by single crystal X-ray diffraction, vibrational spectroscopy (IR and Raman), multinuclear NMR spectroscopy, elemental analysis and DSC measurements. The heats of formation of 1–5 were calculated using the atomization method based on CBS-4M enthalpies. With these values and the experimental (X-ray) densities several detonation parameters such as the detonation pressure, velocity, energy and temperature were computed using the EXPLO5 code. In addition, the sensitivities towards impact, friction and electrical discharge were tested using the BAM drophammer, friction tester as well as a small scale electrical discharge device.

Effect of electronic excitation and ionization on decomposition mechanisms of triaminotrinitrobenzene molecules

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Keywords: triaminotrinitrobenzene molecule; decomposition mechanism; electronic excitation; ionization.

The electronic structures of individual triaminotrinitrobenzene (TATB) molecules in different initial states were calculated by means of density functional theory with the hybrid B3LYP functional and 6-31+G(d) basis set. The ground state, the lowest triplet excited state, positively and negatively charged states of the molecule were taken as initial states. Such initiation mechanisms of decomposition as C–NO2 bond fission and C–NO2 to CONO isomerization with subsequent NO scission were studied quite carefully. All the reaction paths were considered and the activation energies for them were determined. Some other mechanisms of decomposition, which are much less possible, were considered too. All these results were compared with the data obtained for some other nitro compounds molecules in the conditions of electronic excitation and ionization, and a common analysis was performed.

First-principles prediction of metastable nanostructural polymeric nitrogen

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Keywords: polymeric nitrogen; first-principles.

Polymeric nitrogen as potential high density energy materials has attracted great attention. Polymeric nitrogen has been observed in a cubic gauche (cg-N) phase at high pressure and temperature. The cg-N phase, however, transforms back into a molecular nitrogen phase at 42 GPa and is therefore not stable. Stabilization of polymeric nitrogen at ambient conditions remains unresolved and extremely challenging. In this paper, new metastable, nanostructural polymeric nitrogen has been investigated using the first-principles calculations. By wrapping stable polymeric nitrogen zigzag sheets, a single-bonded polymeric nitrogen nanotube is postulated and modeled with structural optimization simulations. This nitrogen nanotube composed of 18 N6 zigzags is metastable as demonstrated by phonon dispersion calculations and molecular dynamic simulations. Like most single-bonded polymeric nitrogen phases, the enthalpy of this nanotube at ambient pressure is higher than that of cg-N. Considering the fact that the lowest enthalpy phase of polymeric nitrogen at ambient conditions is zigzag chain with alternative single and double bonds, novel zigzag jewellery rings of polymeric nitrogen with various radii are further predicted by structural optimization simulations. Two zigzag nitrogen N36 and N48 rings with radii 6.270 and 8.341 Å are arranged into the face-to-face conformation to form one-dimensional tubes. They are metastable at ambient pressure as proven by phonon dispersion spectral and molecular dynamics simulations. Like polymeric zigzag nitrogen, their enthalpies are lower than that of cg-N. This indicates that introduction of mixed bond types in single-bonded polymeric nitrogen phases can lower their enthalpies at ambient pressure and therefore increases the metastability.

Degradation of dinitrotoluenes by bacterial suspension cultures

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Keywords: dinitrotoluenes; biodegradation; Pseudomonas putida; mixed bacterial culture; suspension culture.

This study was focused on the selection of pure bacterial strains being able to degrade dinitrotoluenes (DNT). The effects of environmental parameters i.e., initial pollutant concentration, pH, and the presence of cosubstrates on the rate and efficiency of 2,4-DNT and 2,6-DNT biodegradation were examined. The pure bacterial cultures were isolated from a mixed culture that originated from a long-term contaminated soil near the Explosia plant (Pardubice, Czech Rep.). The degradation experiments were performed in batch aerobic submerged cultivations. The optimal degradation properties were found with Pseudomonas putida at pH 7. These results were compared with those obtained with the mixed culture. It was concluded that the enrichment mixed bacterial culture appeared to be an effective biocatalyst for a remediation of contaminated sites by 2,4-DNT.

With-fracture Gurney model to estimate both fragment and blast impulses

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Keywords: blast; cased; Gurney; fracture; impulse; munitions.

This talk will show that a simple analytical model for exploding cased munitions, developed by R.W. Gurney during World War II, is still capable of further development. The presenter will describe the extensions to Gurney theory that he has recently published, which significantly enlarge Gurney's model to include estimates of blast impulse, in addition to case fragment velocities. The presenter's enlarged Gurney model can also be 'with-fracture'; it can include case material properties under high dynamic loading and high rates of strain, either compressive flow stress of dynamic fracture strain, together with explosive properties, particularly Chapman-Jouget pressure and Gurney energy. The effects of these material properties regarding both performance and safety of munitions can be considerable. Hydrodynamic theory and current and possible future experimental and computational methods useful to the researcher will also be outlined. This work is that of the presenter, quoting corroborative experimental data by other researchers. It is being accomplished by means of analytical calculations, based on Gurney theory, with some Taylor and gas-dynamical theory, experimental data reduction and post-processing of hydrocode output. It is being done at AWE Aldermaston and is sponsored by the UK Ministry of Defence. It has been ongoing since February 2007. A paper in Int. J. Impact Eng. Vol. 36 Issue 2 describes progress up to May 2008.

Key words: Gurney, casing, blast, fracture, impulse, dynamic material properties

Hugoniot of air under kPa and MPa explosive pressures

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Keywords: laser induced breakdown; shock waves; point strong explosion theory; deflectometry.

We present our results on Hugoniot of air under the influence of laser induced miniature explosion, created by focusing a 7 ns, second harmonic of Nd:YAG laser pulse in air. The measurements are carried out from the deflection of a non-absorbing probe beam that gives the information on arrival of shock wave in the region of interest. Shock velocity measured at a fixed distance from the origin of the shock was found to increase with increasing input laser energy, indicating an increase in the shock pressure. Double probe beam deflectometry (DPD) is employed to understand the characteristics of the shock waves (SWs) along the direction of propagation (forward probe) and the direction opposite to the laser propagation (backward probe) from the source of explosion. The study revealed the direction dependent asymmetry in the propagation of SWs revealing the shift in the origin of the SWs with increasing laser energy. At 45mJ of input laser energy, a maximum shock velocity of 11 km/sec, indicating the compression of the air molecules is ob-served while the minimum velocity of 1 km/sec indicating the rarefaction of the compressed layer. The physical parameters associated with SW; Mach, density jump, pressure etc. are estimated using the counter pressure corrected point strong explosion theory (CPCPSET) for SWs. The measured shock velocity, U and the estimated pressure, P released in the explosion, are used to generate the P – U Rankine – Hugoniot jump equation of air.

Theoretical study of adsorption and decomposition of nitroamine on Al(111) surface

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Keywords: nitroamine; Al(111) surface; theoretical study; adsorption and decomposition.

The adsorption and decomposition of nitroamine molecule on the Al(111) surface were studied by DFT method. The calculations employ 4×4 aluminum slab with 3 layers and three-dimensional periodic boundary conditions. There exist both physical and chemical adsorptions associated with different NH2NO2 molecule orientation and particular alumi-num surface sites. For the nondissociative adsorption, the nitro oxygen atom orients to the Al surface. In the case of dissociative chemisorption, the O and N atoms bind with the Al surface. The O and N atoms of broken down N−O and N−N bonds form strong Al−O and Al−N bonds with the neighboring Al sites around the dissociation sites. Moreover, the radical species obtained as a result of N−O and N−N bonds dissociation remain bonded to the surface. The largest adsorption energy is -893.8 kJ/mol. For the dissociation adsorp-tion configurations, a significant charge transfer occurs. The most of charge transfer is 3.04 e from the Al surface to the NH2NO2 molecule. It can be inferred that the aluminum surface is readily oxidized by the adsorbate of nitroamine.

A test to measure long-term high-temperature thermal stability of energetic materials

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Keywords: vacuum thermal stability; ampule thermal stability; high temperature explosives; NONA; TACOT; HMX; RDX; HNS.

We have developed an inexpensive, mercury-free manometric thermal stability test for explosives. The test is especially effective for high-temperature long-duration studies. It overcomes the limitations of the military standard vacuum thermal stability (VTS) test that can only measure up to 11 cm3/g gassing, is temperature limited, bulky and fragile, and uses mercury. In contrast, our ampule thermal stability test can measure up to 300 cm3/g gassing, and test at temperatures up to 350 řC. We routinely run tests for 2 to 2,000 hours. The small size of the test equipment coupled with the ability to store heat-treated ampules for an extended period of time before they are broken and the internal pressure measured, makes it convenient to run a large number of test simultaneously.

Combustion instability of the energetic materials: from microstructures of physical fields to macro-scale properties

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Keywords: combustion instability; micro-structures; liquid-viscous layer; circulating layer; macro-scale properties; C-layer.

Over the last 60 years, a considerable amount of time and money has been spent improving our understanding of combustion instability of the energetic materials (EM). The present state of theory and experiment has not provided a sufficiently strong foundation to provide a complete basis for prediction. Hence there are only a few guidelines available to help designers avoid combustion instabilities. In the last years, researchers have observed the excitation of the spatial periodic micro-structures (SPMS) and the presence of micro-torches at the burning surface of the EM with well pronounced exothermic reactions in the condensed phase and evaporation on the burning surface. Both experiments and theory confirm that the SPMS excitation is a rather universal phenomenon. The electric field micro-structures in the liquid-viscous layer gives the program for formation of the cellular-pulsating micro-structures in the heated-up layer and on the burning surface of the EM. "Wandering" micro-torches on the burning surface causes excitation of the micro-vortex cells – the periodic toroidal vortex micro-structures. In the paper the physical mechanism of excitation of the toroidal-shaped vortex micro-structures over the burning surface is considered. Excitation of the periodic toroidal vortex micro-structures above the burning surface causes increase of the heat flow from the gas phase into the burning surface and, as a result, local increase of the burning rate. Thus, the near-wall periodic toroidal vortex micro-structures form a Circulating layer (C-layer) with a high thermal conductivity, which intensifies the thermal conductivity of the turbulent core of the flow. At increase of the blowing velocity occurs partial destruction of the micro-vortex toroidal structures and reduction of the thickness of the C-layer that leads to reduction of the heat supply to the burning surface. This layer is the basic link between the electric field micro-structures in the liquid-viscous layer and macro-scale properties of the propulsion system. Active con-trolling by self-organizing processes of the spatial-periodic micro-structures in the EM liquid-viscous layer and on the EM burning surface opens possibilities for effi-cient control by the C-layer over the burning surface of the EM. In the paper the modern electro-physical technologies for control by physical-chemical processes in the EM burning wave are analyzed.

Preparation and characterization of glycidyl azide polymer (GAP)

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Keywords: glycidyl azide polymer; epichlorohydrin; energetic binders.

Glycidyl azide polymer (GAP) is an azido-functionalized polymer which burns very rapidly and secures steady state combustion without external heating. The terminal (OH) groups of GAP can be cross linked with an isocyanate. Low molecular weight GAP (Mw from 500-2000) can serve as a plasticizer, while high molecular weight GAP (Mw from 2000-6000) can be used as an energetic binder for composite solid rocket propellant (CSRP) and plastic bonded explosives (PBX's). In this study, GAP binder of high molecular weight was successfully prepared using the modified two-step method. The prepared GAP was characterized by Fourier transformer infra-red (FTIR), elemental analysis apparatus (CHNS) and Gel permeation chromatography connected with light scattering apparatus (GPC-LS). Also, several techniques were used in order to get the final polymer free from moisture as this is very important aspect in using GAP as an energetic binder in CSRP and PBX's. The results show that GAP (Mw 2000-6000) was successfully prepared using the modified two-step method with approximately 98 % yield. Also, the final GAP product after drying was found to have approximately 0.003% moisture content.

Non monotonic detonation velocity in emulsion explosives

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Keywords: detonation physics; emulsion explosives.

Emulsion Explosives (EX), also cited as slurry explosives are generally made of ammonium nitrate aqueous solution emulsified within hydrocarbon mixture of oils and wax and sensitized with hollow glass micro balloons (HGMB) or with air bubbles. This type of explosive is widely used in blasting operations due to its water resistance safety when compared with its detonation parameters and the performance of other common explosives. The EX are arbitrary classified as non ideal explosives because not only its real detonation behavior evaluated by the detonation velocity, pressure, detonation front (DF) curvature or isentropic expansion manifests itself in a much bigger dependence with the explosive charge confinement nature and sizes, when compared with high explosives, but also because that real behavior is significantly different from those expected from equilibrium, steady-state calculations based on the conceptual uni-dimensional Chapman-Jouguet (CJ) model. As the EX are being applied in other areas than rock blasting it is necessary to characterize the detonation behavior of this kind of explosives with much more detail and for much smaller charge diameters than they are being tested up to now. The values of the detonation velocity, the pressure attenuation – P(x) – of DF amplitude in a standard PMMA monitor; manganin gauges pressure-time histories and DF curvature and are show up as a function of the explosive charge porosity and specific mass. All these parameters except the pressure-times histories have been evaluated using the multi fiber optical probe (MFOP) method which is based on the use of an optical fiber strip, with 64 independent optical fibers, connected without any intermediates optics to an electronic streak camera. The MFOP allow a quasi continuous evaluation of the detonation wave run propagation and the assessment to spatial resolved measurements of the shock wave induced in the PMMA barrier which in turns allows a detailed characterization of the detonation reaction zone structure. Moreover, in this paper the effect of the mass concentration of the sensitizing agent – HGMB – on the nonmonotonic dependence of the detonation velocity, of a cylindrical charge, as a function of initial density will be discussed in terms of the finite charge diameter and the width of the chemical reaction zone.

Pressure-cooking explosives: structure determination of energetic materials at extreme conditions

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Keywords: high-pressure; crystallography; RDX; CL-20.

In order to effectively model the behaviour of energetic materials under operational conditions it is essential to obtain detailed structural information for these compounds. In many cases, the crystal structure obtained under ambient conditions is used as the basis for modelling properties at higher temperatures and pressures because structural information if often not available at more extreme conditions. However it is well-documented that such extreme conditions can often lead to substantial changes in intermolecular interactions and molecular geometries, and can even induce phase transitions. It is a requirement therefore that detailed structural information at the molecular level is obtained for energetic materials at extreme conditions if their operational performance is to be more effectively predicted. We have recently structurally characterised the high-temperature, high-pressure polymorph of RDX, allowing us to prove conclusively that the phase of RDX obtained at these extreme conditions (475 K, 4.5 GPa) is not the same as the metastable β-form obtained at ambient conditions, with which it had previously been confused. This finding has significant consequences for the energetics community as a whole since the pressure/temperature regime under which this form, now renamed ε-RDX, is obtained is closer to the conditions typical of detonation, providing an improved starting model for computational studies. The most striking aspect of this experiment however was the recovery of the high-pressure/high-temperature ε-form to ambient pressure at 150 – 220 K. Our studies have recently been extended to obtain high-quality structural data for CL-20 at high temperatures and pressures. As a result of these studies we also present the structure of the high-pressure polymorph ζ-CL-20. These results highlight the unrivalled opportunity for obtaining novel materials that high-pressure studies provide and the exciting prospect of the recovery of further high-pressure phases to ambient conditions. This has been proposed as an effective way of improving performance of energetic materials (such as crystal density, reduced sensitivity, etc) without the need for changing their molecular structure.

Putting the pressure on energetic materials; the structure of zeta CL-20

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Keywords: high-pressure; CL-20; diamond anvil cell; X-ray diffraction.

We have determined the structure of Zeta CL-20 a high-pressure form of CL-20 that trans-forms from gamma CL-20 at 0.7 GPa. As this form is not recoverable to ambient pressures and temperatures we studied this form in situ in a diamond anvil cell with a combination of single crystal and powder x-ray diffraction techniques.

Reactivity of C-NO2 bonds in nitroaromatic compounds: Bond dissociation and disproportionation approach

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Keywords: bond dissociation energy; bond disproportionation energy; nitrobenzenes; nitrotoluenes; detonation velocity.

Homolytic dissociation of C-NO2 bond represents the primary fission process of nitroaro-matic compounds under thermal, impact, shock and electric spark initiation stimuli. Ho-molytic bond dissociation energies BDE(C-NO2) describe the C-NO2 bond fission. Theo-retical calculations of BDEs are substantially influenced by inadequate treatment of elec-tron correlation. Recently the alternative method was suggested to overcome this substan-tial drawback – an isodesmic reaction RC-NO2 + SC-H → RC-H + SC-NO2 where SC NO2 is standard nitroaromatic compound. This reaction is characterized by bond dis-proportionation energy DISP(C-NO2), which inherently cancels the electron correlation effect accompanying homolytic bond dissociation. The bond disproportionation energies DISP(C-NO2) and bond dissociation energies BDE(C-NO2) were evaluated for 11 nitro benzenes and 19 nitro toluenes at DFT B3LYP/6-311+G(d,p) level and correlated with their detonation velocities, D, and with charge of the most reactive nitro group, Q(NO2).

Laser induced breakdown spectroscopy of high energy materials with nanosecond, picosecond, and femtosecond pulses

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Keywords: laser induced breakdown; high energy material; femtosecond.

Laser-induced breakdown spectroscopy (LIBS) has a number of properties that makes it alluring for the detection of explosives, including stand-off detection capability, no constraints on the amount of material, combined with high detection speed [1,2]. Ultrashort laser pulses (picosecond and femtosecond) represent attractive laser sources to design novel and sensitive LIBS systems [3]. The use of short pulses is gaining attention predominantly because it provides certain benefits related to both fundamental studies and delicate analytical problems (e.g. formation of filaments for remote detection). Herein we present some of our results on the LIBS measurements of some high energy materials such as BKNO3, Ammonium Nitrate, Ammonium Perchlorate, and RDX, using ns, ps, and fs pulses. The samples were mixed with KBr and pellets were prepared for spectroscopic studies. Wherever possible as grown crystals (AP,AN) were used for studies so as to eliminate the substrate effects. Nanosecond pulses at 532 nm, picosecond/femtosecond pulses at 800 nm were used for the experiments. The spectra were collected using Ocean Optics 4000 spectrometer. Several features were observed in the spectra, collected without gating and delay, exclusive for each pulse domain. The differences/similarities in the spectra collected using different pulses and details of their origin will be presented in detail.

Trinitrotoluene as a precursor in synthesis of effective azodyes and azopygments

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Keywords: TNT; azodyes; azopygments; synthesis; tautomerism; spectra; quantum-chemical calculations.

The results of investigations of chemical transformations of trinitrotoluene and trinitrobenzene into azodyes and azopygments are presented. About 90 new ammino- and azocompounds were synthezised and investigated by a set of spectroscopic and theoretical methods and tested as acid and dysperse dyes with high resistance to physical and chemical treatments.

Investigation on irreversible expansion of 1,3,5-triamino-2,4,6-trinitrobenzene cylinder

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Keywords: TATB; irreversible expansion; X-ray diffraction; lattice parameters.

The origin of irreversible expansion of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) based PBX is still controversial. In this study, the irreversible expansion of TATB cylinder is investigated. No evident variation of the lattice parameters was observed on TATB crystal and the density of TATB powder decreased by only about 0.02% after it suffered from thermal cycling process at the range from -54°C to 74°C, while the density of TATB cylinder decreased by about 1.0%. It is suggested that the density variation of TATB powder has little contribution to the density decrease of TATB cylinder. Therefore, the increasing interspaces between TATB powder originated from the thermal cycling should be responsible to the irreversible expansion of TATB cylinder.

Investigation on the thermal expansion and theoretical density of 1,3,5-trinitro-1,3,5-triazacyclohexane

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Keywords: RDX; Rietveld refinement; coefficient of thermal expansion; theoretical density.

The linear coefficients of thermal expansion (CTE) and theoretical density are important properties for energetic materials. To obtain the CTE and theoretical density of 1,3,5-trinitro -1,3,5-triazacyclohexane (RDX), X-ray powder diffraction (XRD) and Rietveld re-finement are employed to estimate the dimensional changes in a microcosmic view, within the temperature range from 30°C to 170°C. The CTE of a, b, c axis and volume are ob-tained as 3.07×10-5/°C, 8.28×10-5/°C , 9.19×10-5/°C and 20.7×10-5/°C respectively. Calculated from the refined cell parameter, the theoretical density at given temperature can be obtained. The theoretical density at 20°C(1.7994 g/cm3) is in close match with the RDX single-crystal density (1.7990 g/cm3) measured by density gradient method. It is sug-gested that the CTE measured by XRD could perfectly meet with the thermal expansion of RDX.

Study of physical and chemical properties in some energetic materials from the tetrazole family by the nitrogen NQR

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Keywords: tetrazole; nitrogen 14 nuclear quadrupole resonance; molecular structure; H-bonding; bonding orbitals.

Some recently designed energetic materials are based on the tetrazole ring CH2N4 . It seemed to us worth to get an insight into basic properties of this starting material. We applied the nitrogen nuclear quadrupole resonance (14N NQR) spectroscopy as a method to examine some physical and chemical properties of 5-aminotetrazole and 5-aminotetrazole monohydrate. 14N NQR frequencies and spin-lattice relaxation times were measured at different temperatures between 77K and 300K. Five NQR triplets ν+, ν- and ν0 were found for the five in-equivalent nitrogen atoms in each compound between 0.7MHz and 4MHz. Carr-Purcell based multi-pulse sequences were used to accumulate quadrupole echo signals before the FFT analysis. Assignment of the frequencies to atomic positions was made and the results are analyzed in relation to the molecular chemical bonds and possible H-bonds in the crystal structures. Comparison was made to the previously examined and published NQR spectrum of 1H-tetrazole.

New combinations of energetic compounds for creation propellants for additional propulsion jet systems

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Keywords: energetic compounds; specific impulse.

Proposals to reduce anthropogenic pollution on environment because of separating parts of space launch vehicle and upper stage (boosters) with liquid propellants are under con-sideration. Residual energetic sources that can not be used directly are gasified before be-ing feeding into combustion chamber of gaseous rocket engine. The energy (specific im-pulse) increases due to use of high energy additives (aluminum- and boron compounds containing hydride groups, e.g. aluminum hydride, dimethylaluminum hydride, pentabo-rane) together with classic liquid components (kerosene, liquid oxygen, asymmetric di-methylhydrazine, liquid nitrogen oxide N2O4 etc.). 10% of such energetic additive in-creases the specific impulse value in up to 10 kG•s/kg in comparison with the initial liquid propellant formulation. Therefore the rocket velocity increases considerably (in up to 50 m/s, that is about 10% of initial velocity)

Calculation of combustion, explosion and detonation characteristics of energetic materials

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Keywords: thermochemical codes; energetic materials; combustion; explosion; detonation.

In this work, the thermodynamic code for the determination of the chemical equilibrium composition of a non-ideal heterogeneous system is presented. Computation of combustion, explosion and detonation parameters for some explosives is performed as well as isentropes of products expansion and detonation energy are estimated. Moreover, the non-equilibrium calculations are carried out, in which chemical inertness of one from the components of explosive composition as well as no heat exchange between the component and the detonation products are assumed. At the end, some calculated detonation characteristics are compared with the experimental ones

Vapor Pressure of Energetic Compounds

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Keywords: vapor pressure; correlation; detection.

Vapor pressure is an important thermodynamic property useful in several areas of science and technology. The detection of explosives such as RDX,CL-20, etc require very sensitive sensors, and such sensors need very accurate vapor pressure data. In most cases the very low vapor pressure of these compounds makes it very difficult to measure the data accurately. Limited amount of data exists in the literature for some substance such as RDX but the data differ from author to author. Even in some cases such as TATP which has higher vapor pressures, the data even from a single source varies between multiple measurements. We have undertaken to measure the vapor pressure of some explosives and also correlating the data for predictive purposes.

A theoretical study on pyrolysis mechanism and impact sensitivity of polynitro aromatic compounds

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Keywords: polynitro aromatic compounds; pyrolysis mechanism; impact sensitivity; the first principle.

Polynitro aromatic compounds (including nitro derivatives of benzene, aminobenzenes, phenols and toluenes) are an important category of energetic materials widely used as explosives. Previous works were mainly focused on calculating their structure-performance relations using the semiempirical MO methods. In this study, the title compounds are optimized to obtain their molecular geometries and electronic structures using the first principle at the DFT-B3LYP/6-31G* level. The bond dissociation energies (BDE) of the main bonds for the title compounds have been calculated at the (U)B3LYP/ 6-31G* level. Based on the bond overlap populations and the BDEs, we have discussed their pyrolysis mechanism. It is found that, for the nitro derivatives of benzene and aminobenzenes, the trigger bonds of thermolysis initiation process are C-NO2 bond, and, for nitro derivatives of phenols and toluenes, the activation energies of H-transfer reaction are smaller than the BDEs of all bonds which illustrates that the pyrolysis of the title compounds may be started from the isomerization reaction of H transfer. For example, Figures 1 and 2 present the structures of reactant, transition state (TS) and product of H transfer isomerization reactions of TNP(2,4,6-trinitrophenol) and 2,4,6-TNT(2,4,6-trinitrotoluene), respectively, including the part of the geometric parameters related with the reaction.

In addition, we found that the bond overlap populations (the static electronic structural parameter) and BDEs or the activation energies (the kinetic parameter) all can be parallelly used to identify the stability and the relative magnitude of impact sensitivity for homologous energetic materials, namely, the smaller the overlap population of the trigger bond is, the smaller the stability and the larger the impact sensitivity are. Here, the calculated results from the first principle show that the previous PSBO[4,5] proposed from the semiempirical MO methods is applicable. And the higher the BDE(C-NO2) or the activation energy of H transfer, the less sensitive a compound is. Comparing the static electronic structural and kinetic parameter, it is showed that the former is more convenient and easier to obtain while the latter could be applied more universally for identification of impact sensitivity.

Design and synthesis of new energetic materials

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Keywords: synthesis; energetic materials.

The estimation of the density and detonation properties of C, H, N, O, F explosives is discussed. A simple computer program, "Energy", first developed at the Naval Weapons Center-China Lake in the early 1980's is presented in an updated form. This program allows the rapid calculation of the estimated properties of both known and hypothetical energetic materials. A review of the use of this program in the synthesis of new energetic materials is given. Examples will included polycyclic nitramines such as TNAD and HNIW, heterocyclic nitramines (furazans and tetrazoles)and energetic polymers (poly glycidyl nitrate and poly 3-nitratooxetane).

Theoretical investigation on the thermal decomposition mechanisms of some high nitrogen s-tetrazines

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Keywords: tetrazine; high nitrogen; thermal decomposition mechanism; density functional theory (DFT); ab initio molecular dynamics.

By combining the power of ab initio molecular dynamics method and density functional theory (DFT), the thermal decomposition mechanisms of s-tetrazine molecule and its five derivatives were studied. The present study suggests that: (1) The tetrazine ring can be broken by concerted triple dissociation, concerted double dissociation or single dissociation, which is related with the molecular symmetry, however the triple dissociation is generally dominant in the gas phase. (2) The stability of the tetrazine ring can evidently be strengthened by delocalization between π orbital of the ring and π orbitals or lone pair electrons of the substituent groups including -NH2, -NHNH2, -N3 and -N=N-. (3) The reactions between the substituents and the tetrazine ring (such as H transfer) is not main thermal decomposition pathway and the thermal decomposition mechanisms of the substituent (T)R are similar to those of its simple compound HR. (4) Tetrazines exhibit two principal thermal decomposition modes, which are the ring dissociations and the reactions of substituent groups. If the stability of the substituent is better than that of the tetrazine ring, decomposition occurs first through the ring breaking. Otherwise, the substituent first reacts. The possible bimolecular reactions of DHT were investigated and the reaction energy barrier of the inter-hydrazino hydrogen transfer to loss NH3 was found much lower than that of concerted triple dissociation as the main unimolecular decomposition pathway, indicating it was probably an important thermal decomposition pathway in the crystal phase.

Influences of ignition on burning rates and delay precisions of B/BaCrO4 delay composition

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Keywords: B/BaCrO4 delay composition; delay composition; ignition-cavum; ignition composition.

Different kind ignition compositions and different ignition distance may affect the burning rates of B/ BaCrO4 delay composition. Using B/ BaCrO4(16/84%)and Si/Pb3O4(10/90%) as ignition compositions, changing the boron contents from 3% to 15% in the B/BaCrO4 delay composition, the ignition distance (3.6mm–9.6mm) and ignition structure, then measure the burning rates. The tests results show that the effects of ignition compositions and ignition structure on the burning rates and delay precisions are obvious, while the influence of ignition distance is not so obvious.

Synthesis and crystal structure investigation of novel zinc energetic complexes based on 1,5-diaminotetrazole

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Keywords: synthesis; crystal structure; zinc energetic complex; 1,5-diaminotetrazole.

1,5-diaminotetrazole (DAT) is a kind of high nitrogen-contented compound. Two novel zinc energetic complexes Zn(DAT)2(Ac)2 and Zn(DAT)2Cl2 have been synthesized by reacting 1,5-diaminotetrazole (DAT) with related zinc salts aqueous solution. The single crystals were cultured by slowly evaporating the solvent of the zinc complexes saturated solution. Their crystal structures were determined by X-ray single crystal diffraction analysis. The crystal of Zn(DAT)2(Ac)2 belonged to the monoclinic system, space group Cc, with cell parameters: a=1.7570(3) nm, b=0.7291(15) nm, c=1.4033(3) nm, β=123.66(3)°, V=1.4962(5) nm3, Z=4, Dc=1.712 g•cm-3. The chemical formula of Zn(DAT)2(Ac)2 is C6H16N12O4Zn with Mr= 385.68. In the molecule of Zn(DAT)2(Ac)2, the Zn cation is coordinated with two oxygen from the two acetate and two 4- nitrogen atom of DAT molecule. The lengths of coordination bonds in Zn(DAT)2(Ac)2 are Zn-N of 0.1916(6) and 0.1949(3) nm, and Zn-Cl of 0.2167(1) and 0.2090(1) nm. The crystal of Zn(DAT)2Cl2 belonged to the monoclinic system, space group P2(1)/n, with cell parameters: a=0.5729(11) nm, b=1.1041(2) nm, c=1.5641(3) nm, β=94.83(3)°, V=0.9858(3) nm3, Z=4, Dc=1.562 g•cm-3. The chemical formula of Zn(DAT)2Cl2 is C2H8Cl2N12Zn with Mr= 336.47. In the molecule of Zn(DAT)2Cl2, the Zn cation is coordinated with two chlorine ions and two 4- nitrogen atom of DAT molecule. The lengths of coordination bonds in Zn(DAT)2(Ac)2 are Zn-O of 0.1936(2) nm, and Zn-N of 0.2018(2) nm. In the asymmetric unit, the coordination number of the central zinc(II) cation in the two complexes both are four and the Znic complex display slightly distorted tetrahedron configuration.

Study on the characterization of explosive crystal with μCT

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Keywords: crystal defect; characterization; computed tomography.

The nice and microcosmic structure has close relationship with the properties of explosive crystals. Intragranular defect especially micron defect is one of the key factors that affect the performance of explosive material. The structure of typical crystal explosives (HMX and RDX) is studied with microfocus x-ray industrial volume CT (μVCT) and the explosive crystal defect characteristic are obtained combined with density gradient experiment. The results indicate that micro defects can be quantitatively expressed and the defect dimension and distribution can be distinguishable for different explosive crystal such as normal HMX, RS-HMX and RDX. Component analysis of holes in the crystal shows that there are probably some solvent in the crystals and it is one of the factors that affect the apparent density of crystals.

Studies on dinitrotoluene synthesis using solid state catalyst - H3PO4/MoO3/SiO2

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Keywords: nitration; phosphoric acid; dinitrotoluene; heteropolyacid.

Nitration has been an active area of industrial chemistry, because products of nitration have a lot of applications. A very important nitro-derivative of toluene is dinitrotoluene (DNT). Most of DNT is used mainly in the production of toluene diisocyanate which is used to produce flexible polyurethane foams and glues, lacquers, elastomers and other polyurethane forms. Other uses include the explosives industry. DNT is not used by itself as an explosive, but is converted to trinitrotoluene (TNT), or used as an additive in propellants. It is frequently used as a plasticizer, deterrent coating and burn rate modifier in propellants. It is difficult to obtain dinitrocompounds in one stage by toluene nitration, so DNT is obtained by two-step process. The first step is nitration of toluene to mono-nitrotoluene, and the second step is nitration nitrotoluene to DNT. Toluene is commonly nitrated with the help of a mixture of nitric and sulphuric acids. Using this mixture introduces a lot of pollution (the spent nitration acids) and extra costs (purification and recycling of sulphuric acid). It is necessary to find another catalyst system that could be effective in toluene nitration and gives high yield of dinitrotoluene in one reaction stage. Of interest of these research are the solid acid catalysts that are composed of transition metal oxide (MoO3) and silica gel. These catalysts are activated by using phosphoric acid. The addition of phosphoric acid to these catalysts enhances catalytic properties and gives new compounds and structures on the surface. These types of catalysts were examined in toluene nitration in different conditions. About 20% of DNT is obtained in mild conditions – 2.5 h, ambient temperature with substrates mole ratio 1.5 : 1 (nitric acid : toluene). The very high yield of DNT (85%) was obtained in reaction with only tenfold excess of nitric acid in the same conditions. It was discovered that higher temperature increases reaction yield to 95% in the same reaction time. The way of regeneration of the catalyst system was found. These research show that it is possible to obtain DNT in simple and relatively more ecological way.

Nitrogen-rich salts of N,N'-dinitroguanidine

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Keywords: N,N'-dinitroguanidine; high explosives; crystal structure; detonation parameters; sensitivity.

N,N'-Dinitroguanidine (DNQ) was formed by nitration of N-nitroguanidine using a mixture of HNO3 (100%)/H2SO4/SO3. Nitrogen-rich salts such as ammonium (A), hydrazinium (Hy) guanidinium (G), 1,3,5-triamino-guanidinium (TAG), uronium (U), 5-aminotetrazolium (5AT), 1-methyl-5-aminotetrazolium (1MAT) and 1,4-dimethyl-5-aminotetrazolium (1,4DMAT) were prepared by facile deprotonation or metathesis reactions. All compounds were fully characterized by single crystal X-ray diffraction, vibrational spectroscopy (IR and Raman), elemental analysis and DSC measurements. The heats of formation for the named compounds were calculated using the atomization method based on CBS-4M enthalpies. With these values and the experimental (X-ray) densities several detonation parameters such as the detonation pressure, velocity, energy and temperature were computed using the EXPLO5 code. In addition, the sensitivities towards impact, friction and electrical discharge were tested using the BAM drop hammer, a friction tester as well as a small scale electrical discharge device.

Metal salts of N,N'-dinitroguanidine as colorant and IR illuminants

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Keywords: N,N'-dinitroguanidine; crystal structure; thermal and energetic properties; IR illuminant systems; colorant systems.

N,N'-Dinitroguanidine (DNQ) proved to be a highly energetic material with interesting energetic properties. Alkali and earth alkaline metal salts as well as the copper salt of DNQ can be used for colorant systems. The metal salts were synthesized and characterized by means of vibrational spectroscopy (IR and Raman), elemental analysis, differential scanning calorimetry, and single crystal X-ray diffraction. Sensitivites for impact, friction and electrostatic discharge were determined according to BAM standards. KDNQ and CsDNQ were tested as ingredients in IR illuminants, which were confirmed to be suitable for this application.

Some properties of 3,5-dinitrimino-1,2,4-triazole

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Keywords: high explosives; nitrimines; 1,2,4-triazoles.

A simple method has been offered to obtain 3,5-dinitrimino-1,2,4-triazole (DNRTZ) and salts of DNRTZ. Synthesis is carried out and sensitivity thermal and mechanical initiation of DNRTZ is investigated. Energetic and detonation parameters of DNRTZ were calculated by thermodynamic and simple correlation methods.

Calculation of detonation and shock wave parameters of HTPB-based PBXs

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Keywords: detonation wave parameters; shock wave parameters; HTPB-based PBX.

This paper presents the results of the calculation of detonation and shock wave parameters of cast PBX based on HTPB binder. Compositions based on HMX and RDX, with or without the addition of aluminum and ammonium perchlorate are analyzed. Comparative analysis of calculated parameters to experimentally determined values is performed in order to test the applied mathematical models.

Trinitromethyl bis-triazinyl ethers

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Keywords: bis-triazinyl ethers; substitution of trinitromethyl group; hydroxy-1,3,5-triazine salts.

Synthesis of bis-triazinyl ethers containing trinitromethyl groups was reported. The trinitromethyl derivatives of bis-triazinyl ethers can be synthesized via substitution of trinitromethyl group in 2-amino-4,6-bis(trinitromethyl)-1,3,5-triazines by hydroxy-1,3,5-triazine salts.

New energetic nitrogen rich polymers

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

New energetic nitrogen rich polymers, based on cellulose, were synthesized using common procedures. The point of interest was the introduction of nitramines. The polymers were characterized by) elemental analysis. The energetic properties of the polymers were investigated using differential scanning calorimetry and bomb calorimetric measurements along with calculations using the EXPLO5 software.

Measurement of jet pressure of linear shaped charge

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Keywords: linear shaped charge; jet pressure; velocity distribution.

Paper presents results of laboratory-measured values of jet pressure developed by shaped lined charges. Pressure was measured on contact plane of formed jet and standing target. Distribution of velocity in explosive charge and jet velocity were measured also, in order to determinate dependence function between velocity and jet pressure.Performed researches are base for improved calculation algorithm for determination of jet parameters and linear shaped charge performance.

Development of a bomb calorimetric technique for sensitive explosives

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Keywords: bomb calorimetry; HMTD; heat of formation; primary explosives.

The measurement of the enthalpies of combustion and formation of sensitive explosives by oxygen bomb calorimetry is fraught with technical challenges. Whilst it is impractical to consolidate the pure solid materials into coherent pellets even using a remotely-operated press, both loose powders and pellets deflagrate violently upon ignition in the bomb often damaging the electrode mountings. The use of solid phlegmatizers like benzoic acid or liquid agents like kindling oil often presents other problems, particularly during sample weighing and can lead to scattering of unburned residues in the bomb. In this study low-melting paraffin wax was investigated as a suitable phlegmatizing agent for the sensitive explosive hexamethylenetriperoxydiamine (HMTD). The enthalpy of combustion was measured and the results were compared with the existing published value. The DfH° and DcU° values of HMTD were in reasonable agreement with the published values.

New primary explosive – chlorate(VII) u-4-amino-1,2,4-triazolium-u-dichlorocopper(II)

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Keywords: 4-amino-1,2,4-triazole; complex copper compound; primary explosives.

Salt of chloric(VII) acid and m-4-amino-1,2,4-triazole-m-dichlorocopper(II) was prepared and characterized by elemental analyses, IR spectra and TG/DTA analyses. Sensitivity, detonation velocity and detonator tests were also preformed. The compound has a 1D chain structure in which Cu(II) ions are linked by triazole N1,N2 and Cl- bridges. It is a detonat with initiating performance close to that of lead azide.

Velocity measurements of exploding foil initiators (EFIs) using high speed photography

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Keywords: EFI; exploding foil initiator; initiators; high speed photography.

Exploding Foil Initiators (EFIs) are highly insensitive to mechanical shock and electrical interference, requiring a specific high current pulse for initiation. This allows the use of insensitive secondary explosives, making EFIs a safe and reliable means of initiating explosives. When a high current is passed through the polymer-encapsulated metal bridge, a contained plasma is formed. This causes the film to expand rapidly to form a bubble or shear to form a flyer. This flyer can then impact the secondary explosive and cause initiation. Due to the very high speed at which these systems operate, a streak photography system was used to characterise the behaviour of the polymer film flyers and determine the velocity. This paper will report the effect of bridge size, barrel length and stripline design on flyer speed.

Sensitivity to impact of mixes AP with inorganic components

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Keywords: sensitivity; impact; mixes; ammonium perchlorate.

Till now the set of works on sensitivity to impact of mixes AP with organic (HE, polymers) components is known. The present work we begin a cycle of researches on sensitivity variousdispersed (including nanodimensional) mixes AP with inrganic components – aluminium, oxides aluminium and silicon, carbon and sulphur. The listed components are a part of explosive mixes of different function.

(Nitratomethyl)trimethylsilane and 2,2-dimethyl-1-nitratopropane

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Keywords: natural bond orbital (NBO) analysis; electrostatic potentials (ESP); sigma-hole bonding.

Some properties of two energetic molecules, (nitratomethyl)trimethylsilane and 2,2-dimethyl-1-nitratopropane, were calculated using DFT theory. The structures were fully optimized and NBO analyses carried out at the B3LYP level of theory using a cc-pVDZ basis set. The electrostatic potentials were computed and possible σ-hole bonding discussed.

1-Nitratoethyl-5-nitriminotetrazole derivatives – shaping future high explosives

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Keywords: 1-(2-nitratoethyl)-5-nitriminotetrazole; high explosives; crystal structure; detonation parameters.

1-(2-Nitratoethyl)-5-nitriminotetrazole monohydrate (1) was formed by the reaction of 1 (2 hydroxyethyl-5-aminotetrazole and 100% HNO3. The former one was obtained by alkylation of 5 amino-1H-tetrazole. The byproduct 1-(2-nitratoethyl)-5-aminotetrazolium nitrate (2) has also been characterized and is compared to compound 1. Nitrogen-rich salts such as ammonium (3), guanidinium (4), aminoguanidinium (5), triaminoguanidinium (6) and diaminouronium (7) 1-(2-nitratoethyl)-5-nitriminotetrazolate were prepared by facile deprotonation or metathesis reactions. Most of the compounds were fully characterized by single crystal X-ray diffraction, vibrational spectroscopy (IR and Raman), multinuclear NMR spectroscopy, elemental analysis and DSC measurements. The heats of formation of 1–7 were calculated by the atomization method based on CBS-4M enthalpies. With these values and the X-ray densities several detonation parameters such as the detonation pressure, velocity, energy and temperature were computed using the EXPLO5 code. In addition the sensitivities towards impact, friction and electrical discharge were tested using the BAM drophammer, a friction tester as well as a small scale electrical discharge device.

Study of energetic materials based on the 2,2-dimethyltriazanium cation

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Keywords: 2,2-dimethyltriazanium; monochloramine; HOSA; nitrogen-rich; ion exchange.

2,2-dimethyltriazanium chloride [(CH3)2N(NH2)2]+Cl– (1) and sulphate [(CH3)2N(NH2)2]+2 [SO4]2– (2) were prepared by amination of 1,1-dimethylhydrazine either with one equivalent of monochloramine (3) or by reaction with one equivalent of the sodium salt of hydroxylamine-O-sulfonic acid (Na-HOSA) (4). Exchange of the sulphate and chloride anions in compounds 1 and 2 by energetic anions yielded to the formation of energetic salts based on the 2,2-dimethyltriazanium cation [(CH3)2N(NH2)2]+ on one hand and azide (5), 5-aminotetrazolate (6), 5-nitrotetrazolate (7) and 5,5'-azobistetrazolate (8) anions on the other hand. Compounds 5-8 were characterized by analytical and spectroscopic methods and were investigated as a new class of energetic materials, with possible use in space propulsion.

Qualitative and quantitative analysis of smokeless powders containing new nontoxic stabilizers

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Keywords: smokeless powders; chemical stabilizers; gravimetry; chromatography; infrared spectrometry.

This paper deals with the analysis of smokeless powders containing new stabilizers – epoxidized vegetable oils. These substances should not produce toxic N-nitrosamines during the stabilization of powders. The paper pursues the possibilities of determining of oils and other stabilizers in powders; at the determination of residual solvents; at the modification of samples before analysis; and at the qualitative analysis of oils in smokeless powders.

Ultrasonic investigation on relaxation processes in propellant aging

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Keywords: propellants; ultrasound; relaxation; ageing.

Proposed are ultrasonic investigations on relaxation processes in the frequency range from 1 to 10 MHz of artificially aged single-base (SBP) and double-base (DBP) propellants subjected to laboratory conditions imitating aging of many years. As a main indicator used is the determination of the ultrasonic absorption coefficient. With the single-base propellants, a relaxation transition of 20 years was registered, with it being of local type for 1 and 2 MHz. The double-base propellants contain 15 and 26.5% nitroglycerine (NG), relaxations of various durations at 5 and 15 years were registered with them. With them, the transitions are of cooperative nature. Analyzed were the results obtained and the processes taking place in aging. It has been explained that the ultrasonic absorption increases with the increase of aging products, which leads to structural rearrangement and increase of molecular mobility.

Performance study of 1,3,5-tris(5-amino-3-nitro-1,2,4-triazolyl)-2,4,6-trinitrobenzene - thermally stable explosive

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Keywords: stable explosive; detonation performance; crystal density; heat of formation; impact sensitivity.

Energetic materials including explosives, propellants and pyrotechnics are used extensively for civil applications. There are strong requirements for explosives having good thermal stability, impact and shock sensitivity as well as better performance. The development of thermally stable explosives is a new research field for space programmers, the drilling of deep oil wells etc., which is being actively pursued world-wide. This work introduces a new thermally stable explosive, which can be derived from 5-amino-3-nitro-1,2,4-triazole. This work studies 1,3,5-tris(5-amino-3-nitro-1,2,4-triazolyl)-2,4,6-trinitrobenzene as a new thermally stable energetic compound. Various aspects of detonation performance containing detonation temperature (Tdet), velocity (Vdet) and pressure (Pdet) have been computed by a new computer code. Two new methods are used to calculate crystal density ( ) and solid phase heat of formation (Hf(s)) as two essential inputs of computer code. Also, another new method is used to calculate impact sensitivity (h50).

Synthesis of 2-alkoxy-4,6-bis(trinitromethyl)-1,3,5-triazines

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Keywords: alkylation reaction; 2-alkoxy-4,6-bis(trinitromethyl)-1,3,5-triazines.

Reaction of 2-hydroxy-4,6-bis(trinitromethyl)-1,3,5-triazine silver salt with alkylhalides was studied. It was found the reaction leads to formation of O-alkylation products - 2-alkoxy-4,6-bis(trinitromethyl)-1,3,5-triazines. The structure of 2-methoxy-4,6-bis(trinitromethyl)-1,3,5-triazine was characterized by X-ray analysis.

The scale up process improvement of 1,1-Diamino-2,2-dinitroethane(DADNE)

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Keywords: 1,1-diamino-2,2-dinitroethane; DADNE; preparation.

1,1-Diamino-2,2-dinitroethane(DADNE) is a novel explosive with low sensitivity and high performance. The nitration process of 4,6-dihydroxy-2-methyl pyrimidine was enhanced using organic solvent. The temperature of reaction in nitration step is preferably 20°C-40°C. The reaction time of step is 2 hours. After nitration process, for the hydrolysis of 4,6-dihydroxy-5,5-dinitro-2-dinitromethylene-2,5-dihydropyrimidine, wherein heating reactant is applies in the hydrolysis, thereby solving the safety problem while improving the reaction time of hydrolysis.

Investigation on the characteristic of B/Pb3O4 reaction

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Keywords: thermal analysis; reaction kinetics; B/Pb3O4; delay composition; TG-DSC.

The reaction characteristic of B/Pb3O4 reaction is investigated by DSC-TG, method of Oxygen Steel Bomb and Digital Microscopy. The results show that: The pre-ignition reaction of B/Pb3O4 starts at 370°C; the main reaction zone is around 445°C, and the heat of reaction is 1.6 kJ/g. The results of TG-DSC, Digital Microscopy and Calorimeter results show that the stoichiometry of B/Pb3O4 is about 7%.

Determination of the curing kinetics by NMR

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Keywords: propargyl; curing; kinetics; NMR.

Measurement of the kinetics of curing is an important parameter for manufacturing PBX explosives and propellants. In case of polyurethane formulations, infra-red spectroscopy monitors the disappearance of isocyanates and the formation of the urethane bonds. This method is not usable to observe the reaction between azide and propargyl that leads to triazole linkages. We present a direct determination of the curing kinetics of these new binders by carbon NMR spectroscopy in the bulk mixture without any solvent. Rates of reaction between GAP and different propargyl compounds are compared.

Preparation of RDX particles by ultrasonic atomization

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Keywords: RDX; ultrasonic atomization.

RDX nanoparticles have been widely studied with various energetic materials such as ammonium nitrate (AN), ammonium perchlorate (AP) in order to replace traditional explosive compositions. RDX nanoparticles can be produced in various ways including rapid expansion of supercritical solution (RESS), direct decomposition of hexamine, cold vacuum deposition, vacuum sublimation and wet milling. Those traditional methods have many restrictions such as low production rate, complicated apparatus and uneven size or morphology. In the present work, simple and reproducible production method of RDX nanoparticles was developed by ultrasonic atomization of a solution of RDX. Ultrasound vibration can easily atomize the bulk RDX solution into very tiny liquid droplets and RDX nanoparticles are formed in the hot furnace tube. As experimental variables, solvents, RDX concentration and furnace temperature were taken. The prepared RDX particles analyzed by scanning electron microscopy (SEM) shows that the size of RDX nanoparticles with nearly oval shape is about 500 nm-1μm.

Cooling crystallization of 1,1-diamino-2,2-dinitroethylene

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Keywords: DADNE; cooling crystallization.

For manipulating crystal quality of 1,1-diamino-2,2-dinitroethylene (DADNE), experiments on the crystallization of DADNE by cooling were made as a function of cosolvents(solvent/anti-solvent mixtures), stirring speeds, DADNE concentrations and cooling rates. Particle size, particle size distribution and morphology of DADNE crystals were measured. When N-methyl-2-pyrrolidone (NMP) and dimethylformamide (DMF) were used as single solvent, DADNE crystals were agglomerates with needles or platelets and their yields were about 15-30 %. On the other hand, when cosolvents with water were used, various shapes of DADNE crystals with size of 100-200 mm and yields of 70-80 % were obtained. NMP+H2O and DMAc+H2O were found to be the best candidates to produce cubic DADNE crystals with good surface and narrow particle size distribution.

Nitro compounds based on boron esters

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Keywords: nitroethyl borates; 2,2,2-trinitroethanol; crystal structure; energetic properties.

The reaction of boron oxide with various nitroethyl compounds (2-nitroethanol and 2,2,2-trinitroethanol) furnished the corresponding nitroethyl borates B[OCH2CH2NO2]3, and B[OCH2C(NO2)3]3. A characterization including multinuclear NMR spectroscopy, vibra-tional analysis (IR, Raman) as well as mass spectrometry and elemental analysis was per-formed. The thermal stability was studied using differential scanning calorimetry and the energies of formation were calculated on the CBS-4M level of theory. Furthermore, X-ray diffraction studies were performed and the crystal structure of B[OCH2CH2NO2]3 is pre-sented. The syntheses of the starting materials are described in detail, as well. These boron esters are of interest as possible candidates for high energy density oxidizers and as smoke-free, green colorants for pyrotechnics.

Mechanism of thermal decomposition of some nitro- and oxo-derivatives of pyridine

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Keywords: ammonium 2,3,5,6-tetraoxo-4-nitropyridinate; 4,6-dinitro-2-ethoxy-3-hydroxypyridine; thermal decomposition; mechanism.

Using both theoretical and practical data, the mechanisms of thermal decomposition of ammonium 2,3,5,6-tetraoxo-4-nitropyridinate and 4,6-dinitro-2-ethoxy-3-hydroxypyridine is discussed.

Synthesis and nitration of 1,3- and 1,4-bis(nitrofuroxanyl)benzenes

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Keywords: furoxan; nitration.

The 1,3- and 1,4-bis(3-nitrofuroxan-4-yl)benzenes 1a-c have been prepared by nitrozylation of tetrapotassium salts of 1,3- and 1,4-bis(2,2-dinitro-1-oximinoethyl)benzenes 2a-c with NaNO2 in AcOH and thermally isomerized to 1,3- and 1,4-bis(4-nitrofuroxan-3-yl)benzenes 3a-c. Initial salt 2a-c were in one's turn prepared by an interaction of bis(hydroximoyl) chlorides 4a-c with an excess of dinitromethane sodium salts at low temperature in DMF followed by acidification and treatment with AcOK in MeOH. Nitration of furoxan derivatives 1a-c and 3a-c with the mixture of equal volumes of 100% HNO3 (10 moles) and concentrated H2SO4 at temperature 55-90 oC resulted in mononitro derivatives 5a-c and 6a-c in yields 80-90%. It was found that 5-nitrobenzene derivatives 5a and 6a were obtained at nitration of 1,3-isomers 1a and 3a, 2-nitrobenzene derivatives 5b and 6b – at nitration of 1,4-isomers 1b and 3b, and 4-nitrobenzene derivatives 5c and 6c – at nitration of compounds 1c and 3c.

Detonability of mixtures on a base of various dispersion ammonium nitrate

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Keywords: improvised explosive; ammonium nitrate; detonability; failure detonation diameter.

Quantities of improvised explosive devices on a base of industrial explosives that were applied at criminal incidents or were withdrawn from illegal circulation were reduced on average on 9% during last decade. This tendency is explained in particular by toughening of control under circulation of commercial explosive devices. The most commonly used improvised explosives according to returns of The Forensic Science Center of Ministry of Internal Affairs are mixtures on a base of ammonium nitrate with organic fuels and aluminum powder. Quantitative and qualitative compositions of such improvised mixtures can be various. The most essential question for a criminal case investigator is argument that excepted substance is explosive one. In this connection detonability of the mixtures on base fine-dispersed (particle size was near 20 microns) and granulated ammonium nitrate with some organic fuels and aluminum powder was experimentally investigated. Failure detonation diameters of systems were measured experimentally.

Some properties of HTPB composite propellants

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Keywords: solid composite propellants; ammonium perchlorate; burning rate.

Composite solid propellants of hydroxyl terminated polybutadiene and ammonium perchlorate propellants were prepared. The ratio of medium sized/small sized ammonium perchlorate fractions was kept constant .The effect of adding burning rate catalyst along with the change of the average particle size of fine fraction was investigated. Catalysts are required to enhance burning rates of propellants. Burning rates over a range of pressures from 1 MPa to 5 MP were determined. Burn rates as a functions of pressures were plotted and from the best fit curves the burning rate equation for each formulation was obtained. Mechanical properties (tensile strength, elongation and elastic moduli) of the propellants were also measured.

Sensitivity of energetic materals to effects of electrostatic discharge - effect of distance between test electrodes

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Keywords: energetic materials; electrostatic discharge test; methodology.

In the course of manufacturing of energetic materials (EM) and their subsequent processing, transport, storage and use of their working capacity, these materials are exposed to various risks. Risk situations arise from, among others, exposition of EM's to activation effects of electrostatic discharge. The measure of resistance of EM to effects of discharge is tested by means of instruments of various types, using different methodological approaches, which introduces into this discipline a certain level of difficulty of comparisons of the test data obtained from such different tests. The obtained data depend, inter alia, upon the type of test chamber, the condition and grain size of the sample tested. The submitted methodological paper is focused on investigation of the effect of distance of the flat contact testing electrodes upon the resulting test data evaluating the sensitivity of pyrotechnic compositions containing Pb3O4 as the oxidant.

Applicability of non-isothermal DSC and Ozawa method for studying kinetics of double base propellant decomposition

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Keywords: double base propellant; kinetics; Ozawa method; nitroglycerine evaporation.

In order to determine Arrhenius kinetic constants various experimental techniques and testing conditions have been used. Also, various kinetic approaches and data treatment procedures have been applied, resulting sometimes in considerable disagreement in the values of the kinetic parameters reported in literature. The non-isothermal differential scanning calorimetry (DSC) measurements and isoconversional Ozawa kinetic method are very often use to study kinetics of energetic materials. However, in some cases Ozawa method is used uncritically, i.e. not taking into account some limitations of the method and possible dependence of experimental data on testing conditions. In our previous studies on double base and single base propellants we have shown that testing conditions (sample mass, heating rate, type of sample pan, etc.) may considerable affect kinetic results. An unusual behaviour consisting of existence of a discontinuity and slope change of Ozawa plot, was observed in the case of double base propellants. Such behaviour we explained by sample self-heating effect at faster heating rates and larger samples. In this paper we studied kinetics of decomposition of double base propellants from non-isothermal DSC experiments using unhermetically closed sample pans, and effect of nitroglycerine evaporation on the kinetic results. Kinetics of nitroglycerine evaporation from double base propellants was studied by isothermal thermogravimetry. It was shown by numerical simulation using kinetic data for nitroglycerine evaporation, that at slower heating rates and smaller sample mass nitroglycerine may completely evaporate before DSC peak maximum, resulting in a higher values of the activation energy (173 kJ/mol). At faster heating rates and larger sample mass certain amount of nitroglycerine still exists in the propellant at the peak maximum, resulting in lower values of the activation energy (142 kJ/mol). Although it is evident that the sample self-heating also strongly increases with the heating rates, it seems that the discontinuity point on Ozawa plot coincides with the point of complete removal of nitroglycerine from the propellant sample, which implies that the activation energy obtained for small samples and slow heating rate (173 kJ/mol) corresponds to the activation energy of decomposition of nitrocellulose in double base propellant.

Explosive silver nitrate and perchlorate salts with tetrazole-based ligands

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Keywords: energetic materials; heterocycles; silver; spectroscopic methods; X-ray diffraction.

Methylation of 5-amino-1H-tetrazole (1) gives 1-methyl-5-amino-1H-tetrazole (2) and 2-methyl-5-amino-1H-tetrazole (3). A new family of energetic silver complexes based on ligands 1, 2 and 3 with perchlorate and nitrate anions (10-15) were synthesized and char-acterized by using IR, Raman, and NMR (1H, 13C, 14N, and 35Cl NMR) spectroscopy, ele-mental analysis, and mass spectrometry. The crystal structures of the compounds were de-termined where possible and reveal interesting structural details that are discussed herein. Additionally, differential scanning calorimetry was used to assess the thermal stability of the new salts, which showed excellent thermal stabilities at temperatures up to and above 225 °C. Standard tests were also used to assess the sensitivity of the materials towards im-pact and friction. All the silver complexes showed increased sensitivity values in compari-son with analogous protonated 5-amino-H-1-tetrazolium perchlorate and nitrate salts. Some of these materials have sensitivity values that are comparable to commonly used primary explosives and all of them either deflagrate (12-14) or detonate loudly (10 and 11) on contact with an open flame. Lastly, nitrate salt 11 is easily initiated by thermal shock. It shows reasonably low sensitivity in comparison with other silver salts (e.g., silver azide or silver fulminate), which makes handling it much less hazardous. Compound 11 also has good thermal stability, decomposing at approximately 300 °C, and shows interesting prop-erties as a more environmentally benign alternative to lead(II) diazide in initiation devices for civil and military applications.

Ethylendiamine complexes of the silver and copper salts of 5-nitrotetrazole

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Keywords: nitrogen-heterocyles; transition metals; primary explosives; BAM tests.

Silver 5-nitrotetrazolate (1) and copper(II) 5-nitrotetrazolate 5-nitrotetrazole dihydrate (2) are useful reagents for the synthesis of 5-nitrotetrazole (NT) salts. Both compounds were synthesized and characterized by vibrational spectroscopy (IR and Raman) and differential scanning calorimetry (DSC). In addition, their sensitivity towards friction, shock and elec-trostatic discharge was tested by standard BAM methods. The extremely high sensitivity of both materials makes the transfer of the NT– anion using 1 and 2 hazardous and not suit-able for up-scaling. In order to diminish the hazards involved with the transfer of the ener-getic anion and to render the synthesis of NT salts suitable for an industrial scale the two compounds were stabilized by coordination with a chelating ligand and sil-ver(ethylendiamine) 5-nitrotetrazolate (3) and bis(ethylendiamine)copper(II) 5-nitrotetrazolate (4) were synthesized in high yields. Both stabilized NT– anion transfer re-agents were characterized by analytical and spectroscopic methods. In addition, the crys-tal structure of the ethylendiamine copper complex (4) was determined: Orthorombic Pbca; a = 7.5200(1), b = 14.0124(2), c = 14.7740(2) Å; V = 1556.78(4) Å3). Furthermore, we synthesized triaminocopper(II) 5-nitrotetrazolate (5), which has potential as a more environemtanlly-friendly primary explosive. Lastly, the synthetic potential of the ethyle-diamine adducts 3 and 4 to form energetic NT salts was investigated.

Energetic picrate salts with nitrogen heterocyles

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Keywords: nitrogen-heterocyles; transition metals; primary explosives; BAM tests.

A family of energetic salts based on the picrate anion and several azolium cations were synthesized based either on new methods or literature known procedures. The cations of choice were the following: 5-amino-1H-tetrazolium (1), 1-methyl-5-amino-1H-tetrazolium (2), 2-methyl-5-amino-1H-tetrazolium (3), 1,4-dimethyl-5-amino-1H-tetrazolium (4), 1,3-dimethyl-5-amino-1H-tetrazolium (5), 1,5-diamino-1H-tetrazolium (6), 1,5-diamino-4-methyl-1H-tetrazolium (7), 3,4,5-triamino-1,2,4-triazolium or guanazinium (8) and 1-methyl-3,4,5-triamino-1,2,4-triazolium or methylguanazinium (9). A summary of the 15N NMR shifts for all compounds is given and the proton/methyl induced shifts (PIS/MIS) are compared to the crystal structures. Because hydrogen-bonding plays an important role in determining the density and thus the performance of energetic materials, the crystal struc-tures are discussed in detail. In addition, tests to assess the impact (i) and friction (f) sensi-tivity of the compounds and thermal stability measurements (DSC) were also carried out revealing insensitive compounds (i >40 J, f >360 N) with high thermal stabilities (Td >175 °C). The experimental constant volume energies of combustion were determined using oxygen bomb calorimetry and their validity was checked by way of quantum chemical cal-culation (MP2) of electronic energies. The detonation pressures and velocities of 1 (7795 m s-1, 25.6 GPa), 2 (7343 m s-1, 21.2 GPa), 3 (7213 m s-1, 20.4 GPa), 4 (6876 m s-1, 17.8 GPa), 5 (6846 m s-1, 17.6 GPa), 6 (7864 m s-1, 25.4 GPa), 7 (7492 m s-1, 22.1 GPa), 8 (7495 m s-1, 22.5 GPa) and 9 (7162 m s-1, 19.8 GPa) were predicted using the EXPLO5 code. Lastly, the ICT code was used to predict the decomposition gases of all salts.

Problems in detection of explosives by field asymmetric ion mobility spectrometry (FAIMS)

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Keywords: explosives; IMS.

Countering the explosives threats has been a problem of international concern for many years. A lot of work has been done on bulk detection, but techniques have also been developed to determine traces that may indicate persons or objects recent contact with explosives. For such applications, detection methods which can be made field portable are of high importance. During the last decade ion mobility spectrometry (IMS) has gained a great significance and become a commonly applied technology for the detection of trace levels of explosives in public places and transportation. Commercially available IMS hand held equipment is called explosive vapor detectors. The presented experiments were carried out on portable explosive vapor detector MO-2M produced by Russian company Sibel Ltd. The detection is based on modified IMS technique - the Non Linear Dependence of Ion Mobility (NLDM), also called Field Asymmetric Ion Mobility Spectrometry (FAIMS). MO-2M allows for collection of explosives either in vapor mode or in particle mode. In vapor mode MO-2M directly collects and analyzes air samples in real time. MO-2M is capable of detecting the presence of all military and commercial explosives based on trinitrotoluene (TNT), nitroglycerine (NG), penthrite (PETN) and hexogen (RDX). It can be applied for contact-less, non-intrusive inspection of: persons, luggage, letters and parcels, furniture and vehicles. MO-2M is programmed for reliable detection of four explosives (TNT, RDX, PETN, NG), but for the others the false positive signals are registered. During experiments we determined the detection limits for TNT, RDX, PETN, NG and for the other, rarely used explosives in different temperatures and air humidity. At temperature of 21°C only TNT and NG were detected and correctly identified, RDX was detected when samples were heated to 70°C . The influence of humidity on the sensitivity of MO-2M was also investigated. The parameters were determined for effective detection by measuring different concentrations of selected explosives under different humidity.

Explosive properties of the furazan derivatives

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Keywords: energy of combustion; enthalpy of formation; calorimeter.

Energy of combustion of a furazanotetrazendioxide (FTDO) is measured in the present work on a precision calorimeter. On the basis of experimental data on energy of combustion its enthalpy of formation is got. The knowledge of experimental values of an enthalpy of formation and density has allowed to calculate its explosive characteristics - speed, temperature and pressure of a detonation, heat of explosive conversion. The estimation of parametres of the detonation is executed on the basis of the thermodynamic program of modelling of the detonation considering the equation of a condition of a fluid phase and thermodynamic co-ordinated model of condensed carbon. Comparison of received explosive characteristics FTDO with available experimental data for powerful a HE is carried out

Silver nitriminotetrazolate: a promising primary explosive

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Keywords: primary explosives; nitriminotetrazole.

The synthesis and energetic properties of a potential green primary explosive, silver nitriminotetrazolate is described. When compared with the most commonly used primary explosive, lead azide, silver nitriminotetrazolate exhibits many superior properties including superior thermal, impact and friction stabilities while lacking toxic lead.

A molecular mechanic study of some factors causing high density of nitro compounds

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Keywords: molecular mechanics; charge distribution.

A set of explosives with nitro groups was selected for molecular mechanics calculations of charge density distribution particularly focused on the oxygen atoms of nitro groups. Calculations were done on the basis of accessible X-ray data without structure changes except cases, where hydrogen atoms were not included. Interatomic O...O distances of nitro groups in neighboring molecules were markedly smaller then the van der Waals radii for these oxygen atoms. These atoms have a lower partial charge and therefore lower repulsion forces and higher dispersion forces. The mutual repulsion and dispersion interactions were calculated on the base of experimentally derived structures for nitro groups in Compass force field. Moreover, the presence and power of hydrogen bonds, both connecting atoms in the individual molecules and connecting molecules in the crystal, results in a density increase of the substance. Obviously, both these factors probably contribute to the unusually high density values of poly-nitro compounds.

The usable parameters of PBX containing FOX-7

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Keywords: PBX; FOX-7.

In this paper, usable parameters of Plastic Bonded Explosives containing FOX-7 and hexogene or octogene are presented. The working capacity of PBX was measured by determination of intensity of blast wave. During the experiments, the overpressures blast wave and positive phase impulse were determined. The tests showed, that these two parameters decrease with growth of the FOX-7 content, however the decrease of impulse is smaller than the decrease overpressures blast wave. In this work, the shaped charges of typical construction which is used to perforation in oil mining were tested. The penetration capacity of steel plate by tested shaped charges was determined. The results of tests show that penetration of tested charges is on the same level with charges containing RDX. Penetration of charges including mixtures of FOX-7/RDX was in the 117÷116 mm range, however for FOX/HMX it was 117÷127 mm.

Investigation of tetrakis(2,2,2-trinitroethyl) orthocarbonate (TNEOC) as high energetic dense oxidizer (HEDO)

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Keywords: oxidizer; trinitroethanol; sensitivity; DSC; crystal structure.

Tetrakis(2,2,2-trinitroethyl) orthocarbonate (1, TNEOC) was synthesized by the reaction of tetrachloromethane with four equivalents of trinitroethanole and catalytic amounts of iron trichloride. Compound 1 was fully characterized by single crystal X-ray diffraction, vibrational spectroscopy (IR and Raman), multinuclear NMR spectroscopy, elemental analysis and multi-temperature DSC measurement. Due to the positive oxygen balance, the suitability of 1 as a potential oxidizer in energetic formulations has been investigated and discussed. In addition, the heat of formation of 1 was calculated using the atomization method based on CBS-4M enthalpies. With this value and the experimental (X-ray) density, several detonation parameters such as the detonation pressure, velocity, energy and temperature were computed using the EXPLO5 code. In addition, the sensitivity towards impact, friction and electrical discharge was tested using the BAM drop hammer, a friction tester as well as a small scale electrical discharge device.

Introduction DNU as a new energetic compound to improve performance of solid propellants

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Keywords: dinitrourea; energetic compounds; detonation temperature; heat of formation; computer code.

The search for new energetic compounds with high content of energy and desirable properties is one of the major challenges to the chemical industry. In this work, a new energetic compound N,N'-dinitrourea (DNU) will be introduced, which is suitable its application in solid propellants and gas-generator systems. A new theoretical model is used to calculate the condensed phase heat of formation of this compound. The specific impulse (Is) of DNU has been computed by complex computer code ISPBKW and compared with those of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) and octahydro-1,3,5,7-tetranitro1,3,5,7-tetrazocine (HMX) as two common energetic oxidizers in solid propellants. Furthermore, detonation temperature (Td) and oxygen balance (O.B) of DNU has been computed and compared with those of RDX and HMX.

Analysis of heat transfer in explosives

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Keywords: explosives; heat transfer; simulation.

The heat transfer in explosives can be described by Fourier equation with the additional term for the heat generated by decomposition of the explosive. This equation can be solved numerically. E.g. an ignition temperature during a slow cookoff test can be calculated if is the explosive properly characterized. The density, thermal conductivity and heat capacity, together with the description of decomposition reaction kinetics (heat of reaction, activation energy, preexponential factor and reaction model) are to be known to characterize the material. However an importance of these individual parameters on the solution has not been published in a self-contained form.

The influence of the individual material properties on the solution is studied. As a standard, a simulation of the slow cookoff test of Semtex 1A using one dimensional finite difference method was used. The results of the simulation corresponds to experimental data. The material parameters were varied between 50 and 200% of their original value (the ranges for density and activation energy were scaled down to obtain physically realistic values). The influence of these variation on the calculated ignition temperature is evaluated and discussed.

Probit analysis in evaluation of explosive's sensitivity

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Keywords: probit analysis; sensitivity; friction; impact.

The sensitivity of explosives to various initiating events has a shape of sigmoidal curve. In standard sensitivity tests one point on this curve is sought most often the 50% initiation probability level. The most common method for its determination is the up-and-down method. The whole sensitivity curve can be obtained by conducting large number of trials at all levels or more effectively by probit analysis. The usage of probit analysis, improvement the precision of the results and comparison with the up-and-down method is demonstrated on the example of determination of sensitivity to friction.

Crystallization and mechanical stirring of TEX and HNIW

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Keywords: mechanical stirring; TEX; HNIW.

In this paper, the methods of crystallization and mechanical stirring of TEX (4,10-dinitro 2,6,8,12-tetraoxa-4,10-diaza-isowurtzitane), HNIW (CL-20, 2,4,6,8,10,12-hexanitro 2,4,6,8,10,12-hexaaza-isowurtzitane) are presented. The aim of work was to obtain spherical crystals of mentioned materials. Several solvents for mechanical stirring were checked. The influence of various parameters on mechanical stirring was investigated The particle size distribution and the density for the obtained crystals are presented

1-Dinitromethyl-3-nitro-1,2,4-triazoles thermal decomposition under non-isothermal conditions

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Keywords: thermal decomposition; geminal dinitrocompounds; steric effect; characteristic temperature; correlation.

The thermal decomposition of substituted gem-dinitromethyl-3-nitro-1,2,4-triazoles in liquid phase is investigated by the method of derivatography using IR-spectroscopy. The activation parameters of some compounds are determined. Using differential-thermal analysis the characteristic temperatures are established. It is shown that steric effect of a-substituent at gem-dinitromethyl group influences on the decomposition rate and the characteristic temperatures. The reactivity of investigated compounds is analyzed and the correlation dependences are found which have a prognostic force.

Salts of 2-methyl-5-nitroaminotetrazole – low sensitivity secondary explosives

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Keywords: 2-methyl-5-nitriminotetrazolate; secondary explosives; crystal structure; detonation parameters; sensitivity.

2-Methyl-5-nitroaminotetrazole (1) was formed by nitration of 2-methyl-5-aminotetrazole. 2 Methyl-5-aminotetrazole was obtained by methylation of sodium 5-aminotetrazolate. Nitrogen-rich salts such as ammonium (2), hydrazinium (3) guanidinium (4), 1 aminoguanidinium (5), 1,3-diaminoguanidinium (6), 1,3,5-triamino-guanidinium (7), uronium (8), and 1,3-diamino-uronium (9) 2-methyl-5-nitriminotetrazolate were prepared by facile deprotonation or metathesis reactions. All compounds were fully characterized by single crystal X-ray diffraction, vibrational spectroscopy (IR and Raman), multinuclear NMR spectroscopy, elemental analysis and DSC measurements. The heats of formation of 2–9 were calculated using the atomization method based on CBS-4M enthalpies. With these values and the experimental (X-ray) densities several detonation parameters such as the detonation pressure, velocity, energy and temperature were computed using the EXPLO5 code. In addition, the sensitivities towards impact, friction and electrical discharge were tested using the BAM drop hammer, a friction tester as well as a small scale electrical discharge device.

Novel nano-scaled electrocatalysts for hydrogen evolution with reduced loading of precious metals

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Keywords: composite catalyst; activated multiwalled carbon nanotubes (MWCNTs); hydrogen evolution reaction (HER); Ru; Pt; Co; TiO2.

The aim of this work was to reduce the loading of precious metals in electrodes for hydrogen evolution. The investigated electrocatalysts contain mixed metallic phase (20% Pt or Ru and the rest 80% Co), TiO2 and activated multiwalled carbon nanotubes (MWCNTs). For comparison, catalysts with pure metallic phase were prepared (Ru, Pt, Co). Structural characterization was performed by XRD, TEM, and FTIR methods. It was shown that Co and Ru particles are very small, near 2 nm, while Pt near 12 nm. Pt particles in the mixed electrocatalysts have decreased up to 3-4 nm. Pure and mixed Ru-systems have shown the best performances, as result of the very small particles, i.e. high developed surface area of the active catalytic phase. In the Pt-based systems, the catalyst with mixed CoPt metallic phase (only 20%Pt) has showed very close catalytic activity to the corresponding catalyst with pure Pt metallic phase (100% Pt). This is result of significantly smaller particle size of Pt and Co in the mixed metallic phase related to the particle size of pure Pt phase. The smaller amount of Pt was compensated with considerably higher surface area of the active catalytic centers.

The study of gun shot residues from the cartridge in the dependence on the gun barrel length

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Keywords: gun shot residues; ammunition.

Current trends in the construction of ammunition have been aimed at the development of new materials, which should represent a reduction of toxic risk for a gunner and his surroundings. Currently, the research of gun shot residues, on the basis of which we can presume the suitability of the used material in terms of toxicity, constitutes wide and very interesting problems. There are directives in many countries, which partially define requirements for „nontoxic“construction parts of the cartridge and especially for the ignition composition and propellant. A problem arises for designers and developers to solve and realize these requirements and so this object of the construction of ammunition is studied at many professional workplaces. Particularly, we have been dealing with the study of gaseous gun shot residues for 6 years. The methodology of a catch gun shot residues has been processed and verified and a huge database of results has been obtained by various combinations of ignition compositions and propellants for the cartridge 9 mm Luger during this period above all. In this paper, we present several results of the influence of gun barrel length on the quality of gun shot residues for the cartridge 9 mm Luger.

The obtaining the crystallites the CL-20 of reduced sensitivity

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Keywords: CL-20; energetic materials; crystalization.

Development of energetic materials with improved performance and reduced sensitivity characteristics is a major goal in the area of high energy materials. CL-20 or hexanitrohexaazaisowurtzitane is a relatively new energetic material that exhibits higher density and heat of formation than RDX and HMX, the conventional energetic nitramines. These superior properties are due to its unique caged structure with characteristics of high density, strained ring, and high branching, respectively. CL-20 has several different crystal polymorphs including the α, β, ε, γ polymorph. The ε polymorph has high energetic performance, high density, and low sensitivity compared to the other polymorphs, which makes the ε polymorph more desirable for use in propellant and weapons systems. The material purity, crystal polymorphism, morphology and crystal quality can greatly influence the sensitivity of energetic crystals. Therefore, crystallization processes are suitable techniques to improve the quality of CL-20, especially to decrease the sensitivity. Precipitation by an antisolvent is the suitable method of obtaining the crystallites the CL-20. When the antisolvent is added to the solution, solubility of the solute decreases and the solution becomes supersaturated. Upon reducing the solubility a supersaturation is created which induces the nucleation of crystals. The various crystallization parameters such as temperature, antisolvent addition rate and agitation are adjusted to get the required final crystal size and morphology. The solvent–antisolvent ratio, time of crystallization and yield of the product are the key factors for controlling antisolvent based precipitation process. This study was undertaken to identify the parameters that control ε- CL-20 sensitivity: crystal shape and dimensions as well the crystal grains distribution. The crystallizations were carried out with change of parameters such how: the kind of the antisolvent not described yet, time of antisolvent addition, speed of stirring, resulting in the obtained ε- CL-20 grains mentioned above properties, which strongly influence their sensitivity measured by Peters and Kast methods.

Polynitroderivatives of alkoxy- and alkylendioxy- benzenes: potential HEMs and precursors of new energetic materials

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Keywords: polynitroderivatives; HEMs; synthesis; reactions; nitration.

Several di-, tri- and tetranitroderivatives of alkoxy-, dialkoxy- and cyclic alkylendioxyben-zene derivatives were synthesized by nitration of starting compounds in different condi-tions and their properties were compared to already known 2,4,6-trinitroanisole and TNT. Their potential as HEMs or precursors of new energetic materials is discussed.

Synthesis of energetic materials, containing benzimidazole core

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Keywords: benzimidazoles; nitrocompounds; nitramines; azides; picrylderivatives.

A number of azaheterocyclic nitrocompounds (including 2,4-dinitro- and 2,4,5- trinitroimidazoles) are already known as perspective high energy materials (HEMs). Benzimidazole derivatives are almost not studied in this aspect. The main goal of the present work was the preliminary investigation of the synthesis and some characteristics of a numerous di- and poly- nitrocompounds, containing benzimidazole core bearing “explosophoric“ nitramino-, hydrazino- , azido- and other functional groups. Several compounds among them have been selected on the basis of acceptable oxygen balance (OB) and other characteristics. Selected compounds may be potentially interesting for HEM application.

Organic nitrates and nitramines: synthesis, electrochemistry and cytotoxicity studies

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Keywords: nitrates; nitramines; preparation; voltammetry; cytotoxicity.

Laboratory scale quantities of a series of organic nitrates and nitramines were obtained by nitration with dinitrogen pentoxide in dichloromethane medium. Twenty seven synthesized compounds were explored by voltammetry methods and their cytotoxicity for mice splenocytes was evaluated. N.N'-Dinitropiperazine, DINA and hexandiol-1,6-dinitrate were determined as some of the most toxic compounds. Several compounds having non-planar cyclic, bicyclic or cage structures (IHN, TNAD, DINGU, TEX) were found as less toxic, possibly due to poorer penetration through the cell membrane.

Investigation of thermobaric layered charges

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Keywords: thermobaric explosives; blast wave characteristics.

The research on detonation of SFAE-type charges was carried out. Charges which composed of a cylindrical layer of a mixture of ammonium nitrate and aluminium powder surrounded the phlegmatized RDX were tested. To trace the curvature of a shock wave in the external layer, X – ray photography was applied. The pressure blast characteristics and the light output of explosion cloud was investigated in the bunkers of different size and level of opening (a ratio of holes' surface to the total bunker surface). Amplitudes and impulses of the incident waves and the impulses of the total overpressure recorded in the specified time duration were analysed. The obtained results can be helpful for the construction of thermobaric layered explosives.

Dft studies on novel energetic materials: (e)-2,4,6-trinitro-n-(2,4,6-trinitrobenzylidene)benzenamine and its isomers

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Keywords: high explosives; polynitro compounds; DFT; ballistic properties.

Some novel energetic materials have been designed starting from molecule (E)-2,4,6-trinitro-N-(2,4,6-trinitrobenzylidene)benzenamine (I) , which is isoconjugate with HNS. It differs from HNS by having an aza-substitution (centric perturbation) at the olefinic corbon. The other structures are constitutional isomers of (I). By using DFT [B3LYP/6-31G(d)] approach various MO and ballistic properties of these structures have been calculated and compared with values of HNS and HNAB which are related to (I).

Explosion hazard of aromatic mononitrocompounds that used in a pharmaceutical industry

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Keywords: mononitrocompounds; explosion hazard; thermal decomposition; exothermic effect.

Two nitroccompounds, p-etoksi-m-nitroacetianilid and m-nitro-aminofenetol, are the semiproducts of the synthesis of new pharmaceutical: afobasol and bradisol. Explosion hazard of mononitrocompounds is widely considered in scientific literature and it was established, that the mechanism of their decomposition is similar to decomposing of polynitrocompounds. Thermal decomposition of these substances was studied by means of method DTA in opened and closed crucibles. Investigation in opened crucibles has shown that substances were easily flying and at heating to 250 oC they are evaporated completely. For modeling conditions of the heating in closed capacities crucibles with covers have been applied. The behavior of substances in closed crucibles has changed. The weight decrease begins at higher temperatures (239 and 286 oC) and it is connected with destruction of the weakest bond in structure - Sar-NO2. Decomposition of the m-nitro-aminofenetol and p-etoksi-m-nitroacetianilid are accompanied with exothermic effects, 378,0 and 985,3 kJ/kg, corr. Thus, considered mononitrocompounds can show explosive properties at heating in the closed capacities.

Detonation parameters of water-impregnated explosives containing various aluminum powders

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Keywords: water-impregnated explosives; aluminum powders; detonation; electromagnetic technique.

Water-impregnated metal-containing compositions are high-performance and safe explosive materials characterized by very low levels of mechanical and heat sensitivity. The main objective of this work is study of effect of aluminum particle size on detonation parameters for gelled water-impregnated aluminum-containing explosives (WAE). The water-gel matrix consisted of ammonium nitrate, sodium nitrate, water and polyacrilamide. Pigment grade flaked aluminum powder PAP-2 and aluminum powders of various type: ASD-4, ASD-1 and PA-3 were added to water-gel matrix. Particle size of aluminum powders in formulations varied from 5 to 150 mcm. Measurements of profiles of particle velocity vs. time, u(t), and detonation velocity, D, for investigated compositions carried out by means of electromagnetic technique. The dependencies of detonation parameters on aluminum particle size, on the charge diameter and density were determinated.

Viscoplastic behavior of solid propellants

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Keywords: solid propellants; viscoplastic behaviour; experimental tests.

In the paper an initial attempt to the experimental analysis of viscous effects, characteristic for homogeneous solid rocket fuels is proposed. For this reason uniaxial tensile experiments, carried out on dumbbell homogeneous solid propellants have been chosen. Laboratory tests have been carried out on INSTRON tensile testing machine. Research schedule involved destructive tensile tests with various strain rates. Three different values of strain rates have been taken into considerations. Experimentally obtained hardening curves are presented in suitable diagrams. Basing on obtained results, authors confirm the viscoplastic behavior of previously mentioned materials. Essential impact of the applied strain rate on the position of experimental hardening curves is observed. Acquired results are the base for the further stage of investigations of homogeneous solid propellants – modeling of their physical properties. The global aim for authors is to establish connections between the loading history of solid propellant (thermal and mechanical) and its ballistic properties. In this work authors are approaching the first stage – collecting the experimental data for the establishing a suitable constitutive model for solid rocket fuels.

Analysis of influencing factors of mortar projectile reproduction process on fragment mass distribution

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Keywords: reproduction process; mortar projectile; statistical analysis.

This paper deals with high explosive projectile reproduction process over several years of monitoring and testing its fragmentation characteristics. Experimental data used in analysis were obtained using PIT tests in our country. Many fragmentation tests (more than 80 projectiles) were conducted with 19 different production series of projectile mortar projectile 120mm, in a time span of over three years. Number, mass and fragments shape of each fragment mass group are determined using the PIT test. In PIT test, warhead is detonated in closed space, filled with sand. After the fragmentation of warhead, fragments are obtained from the sand. Mass and shape of fragments are determined, and fragments are classified by their mass groups. Number of methods are available for prediction of fragment mass distribution, such as Mott or Held method. Authors tried to find appropriate influencing factors on reproduction process, such as variation of explosive main charge detonation parameters, mechanical properties of warhead case material – such as steel ultimate tensile and yield strength, as well as production process variations. Statistical variation parameters (min, max, range, median, std. dev, and variance) were determined in order to clarify the quantitative difference between individual test results and their impact on fragment mass distribution.

Dispersion of PGU-14 ammunition during air strikes by combat aircrafts A-10 near urban areas

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Keywords: DU ammunition; dispersion; airstrikes.

Nineteen air strikes onto seven target locations in Bosnia and Herzegovina were carried out by aircrafts A-10, using ammunition PGU-14. During these air strikes, 10086 pieces of PGU-14 were fired, strafing such targets as armored vehicles, trucks and bunkers. Exact locations of targets and PGU-14 ammunition quantity, which were spent for six attacks, are still unknown. But for one target, which was located near Sarajevo at suburb settlement Hadzici it was possible to collect more information. Two targets, an ammunition depot and the tanks and armored vehicles maintenance facility, were attacked at the Hadzici location. During the five air strikes, 3400 DU projectiles of PGU-14 ammunition were fired onto these targets. One of the targets was located within the urban part of the settlement, while another one was at suburb part of the settlement. Research points to very large number of unknown locations and uncomplete data on quantity of ammunition PGU-14 that was fired onto individual targets. There is disproportion between points of impact of DU penetrators into hard surfaces and number of located penetrators (ricochet effect), which in longer time period increases health risks for civilian population. Purpose of this paper is to perform an estimation of the dispersion zone with ground-penetrated projectiles PGU-14 using ballistic trajectory simulation for aircraft gun GAU-8/A and ammunition PGU-14 fired from aircraft A-10 and available input data such as aircraft velocity during the air strikes and ballistic performances of projectile PGU-14. In order to obtain final dimension of the hit dispersion pattern, theoretical results are corrected by using a dispersion figure gained from a real combat action. For this purpose, a detailed analysis of video-records (1995-2008 years) of combat actions carried by aircrafts A-10 on area targets without anti-aircraft protection and under conditions of very intensive anti-aircraft fire. Hit probability is determined on the base of US researches, which were performed during 1979 and 1980, in order to simulate attacks on Russian tanks under low attack angles. Based on the estimated number of hits for armored or other hard targets, it is possible to approximately determine dispersion of PGU-14 ammunition during air strikes in target zone near urban areas.

TATB crystal morphology controlling by recrystallization

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Keywords: TATB; recrystallization; non-solvents; crystal morphology.

1,3,5-triamino-2,4,6-trinitrobenzene (TATB) is a widely applied insensitive explosive. However, the TATB-based PBXs commonly present anisotropic expansion and deformation, which usually bring some negative effects on the application of TATB. It is predicted that PBXs packed from spherical TATB crystals may have less anisotropic expansion and deformation. In this paper, TATB crystals with different morphology were obtained by means of high temperature non-solvents recrystallization. That means TATB was dispersed into DMSO and heated to a higher temperature to make it dissolv, and then water, as a non-solvent, was added to the solution with other ingredients controlled. It is shown that the crystal morphology is strongly affected by stirring rate and the proportion of water.

Transformation of aluminium at explosion of its mixtures with TATP and HMTD

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Keywords: peroxides; TATP; HMTD; aluminium; aluminium hydride; aluminium oxide; HMX; synthesis; explosion at impact.

Mixtures of benzoyl peroxide with aluminum and aluminum hydride and HMX have been under investigation at past works. It was shown that aluminium and aluminium hydride may serve as indicator of thermodynamic contribution of energetic material. Theirs behaviours at explosion are quite different and it also was shown in previous work. It was also shown that difference between organic peroxides and energetic materials is in chemical reactions at explosion. As we supposed in previous work formation of 2 forms of aluminium oxide at explosion of mixtures HMX/AlH3, opposed to mixture HMX/Al where aluminium in form of aluminium powder PAP-2 turn into only 1 form of aluminium oxide, connects with different aluminium and aluminium hydride behavior at explosion. Mixtures of TATP and HMTD with aluminium and aluminium hydride were studied in this work. Results of present work have been compared between each other and also with results of our previous work.

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