ON MATERIALS' CAPABILITY TO DETONATE

A.N. Dremin
Institute of Problems of Chemical Physics Chernogolovka, Moscow Region, 142432, Russia

Abstract:
The idea of how to determine the composition of mixtures of liquid explosives with inert diluents and solutions of solid explosives in inert solvents which are still capable to detonate has been introduced. It has been demonstrated experimentally with nitromethane/acetone mixtures and diethanolnitramindinitrat/acetonitril solutions that the most weak composition still capable to detonate is that which detonation's CJ pressure is still larger than the minimum shock pressure necessary to initiate the detonation. Considerations have been proposed on conditions at which so called gasless detonation could be realized theoretically.
NTREM, PARDUBICE, 2004 page 13-22

NEW HIGH EXPLOSIVES AND PROPELLANTS BASED ON BIURET AND TETRAZOLE COMPOUNDS

T.M. Klapötke*, G. Holl, J. Geith*, A. Hammerl* and J. Weigand***
* Department of Chemistry, University of Munich, Butenandtstr. 5-13 (D), D-81377 Munich Germany)
** Bundeswehr Research Institute for Materials, Fuels and Lubricants, Swisttal-Heimertsheim; Großes Cent, D-53913 Swisttal (Germany)

Abstract:
The synthesis of energetic, non-nuclear materials for possible military application has been a long term goal in our research group. Modern high-energy-density materials (HEDM) derive most of their energy either (i) from oxidation of the carbon backbone, as with traditional energetic materials or (ii) from their very high positive heat of formation. Examples for the first class are traditional explosives such as TNT, RDXand HMX. Modern nitro compounds such as CL-20, TEX or the recently reported hepta-and octanitrocubanes possess very high densities and have enhanced energies due to substantial cage strain. The most recent and most exciting members of the second class of compounds are 3,3'-azobis(6-amino-1,2,4,5-tetrazine) and various salts which are based on the 5,5´-azotetrazolate dianion, which derive most of their energy from their very high positive heats of formation. The heavy metal salts of 5,5´-azotetrazolate, particularly lead 5,5´-azotetrazolate dihydroxide, have been investigated for use as initiators. The ammonium, guanidinium and triaminoguanidinium salts of 5,5´-azotetrazolate were found to be powerful, yet smokeless gas generators. Since in general, tetrazole derivatives are very useful building blocks in the chemistry of highly nitrogen-rich compounds, in this contribution we report on the synthesis and characterization of several tetrazole based energetic materials with up to and over 90% nitrogen.
The synthesis, NMR spectroscopic characterization and structure determination of highly explosive tetrazole azide, a very nitrogen-rich material (88.3% N) is reported. The computed electrostatic potential suggests a pronounced shock and friction sensitivity which was confirmed experimentally. Quantitative valence bond (VB) calculations were performed for the most important 21 VB structures in order to obtain the structural weights and to obtain an assessment for the importance of the various individual VB structures considered.
The synthesis, reactivity and physical properties of new nitrogen-rich, highly energetic materials is presented.
Examples of nitrogen-rich compounds with up to 95% nitrogen content by weight include hydrazinium azide hydrazinate, $N_2H_5^+N_3^-\cdot N_2H_4$ (91.5 % N) and trintirotriazidobenzene, C6(N *3)3(NO2)3. Also presented are new, highly energetic tetrazole derivatives and derivatives oftetrazene.*
The heats of combustion (ΔHcomb.) of dinitrobiuret (DNB) and diaminotetrazole nitrate (HDAT-NO3) were determined experimentally using oxygen bomb calorimetry: $\Delta H_{comb.}$(DNB) = 5195 ± 200 kJ kg^{-1}, $\Delta H_{comb.}$(DAT-NO_3) = 7900 ± 300 kJ kg^{-1}. The standard heats of formation (ΔH°f) of DNB and HDAT-NO3 were obtained on the basis of quantum chemical computations: ΔH°f(DNB) = - 353 kJ mol^{-1}, - 1829 kJ kg^{-1}; °f(HDAT-NO3) = + 254 kJmol^{-1}, + 1558 kJkg^{-1}. The detonation velocities (D) and detonation pressures (P) of DNB and HDAT-NO3 were calculated semiempirically: D(DNB) = 8.66 mm μs^{-1}, P(DNB) = 33.9 Gpa; D(DAT-NO_3) = 8.77 mm μs^{-1}, P(HDAT-NO_3) = 33.3 Gpa.
Integral to this research are investigations concerning the explosive nature and safe-handling of

such compounds. The sensitivity of the compounds towards heat, friction and electrostatic shock have been both experimentally (drop hammer, steel sleeve and firing tests) and theoretically investigated (calculation of electrostatic potential surfaces).
Possible applications for these energetic materials will be highlighted, in particular with respect to new detonators and rocket propulsion systems.
NTREM, PARDUBICE, 2004 page 23-34

NEW SAFETY THINKING APPLICABLE TO EM SYNTHESIS AND MANUFACTURE

H.J. Pasman and J.F. Zevenbergen
Delft University of Technology, Faculty of Applied Sciences, Explosion Group Julianalaan 136,2628 BL Delft, Netherlands

Abstract:
The occurrence of major accidents in the chemical process industry has over the years stimulated world wide safety thinking. This resulted also rather recently in interesting new concepts in the approach to design and the control of operation of processes with hazardous materials. A practical concept applicable in many situations is the layer of protection analysis. This kind of top down barrier thinking encompasses both technical and organisational measures and is very suited for risk control both in the laboratory and in the case of industrial installations. It involves the user and his management and can optimise cost-benefit. It can be used in new design, but also for installations that have been operated already for years. Thinking starts of course with the question what are the risks and can these be prevented. The inherent safer approach offers a number of check list items which can be checked off. Improvements can semi-quantitatively be measured by indexing. Of course with energetic materials inherent safer working has its limitations, but sometimes by selecting different solvents, other installation lay-out etc. considerable improvements can be made. Subsequently independent layers of protection are defined. Independence is not easy to realise, but is a crucial condition. In a second part specific hazards of energetic materials are highlighted .This is covering the initiation and explosion severity of energetic materials themselves, the process runaway risk when manufacturing them and the health hazards solvents may present.
NTREM, PARDUBICE, 2004 page 35-50

INFLUENCE OF TAMPING ON PERFORMANCE OF LINEAR SHAPED CHARGES

Z. Akštein and L. Říha
Research Institute Of Industrial Chemistry Explosia a.s., 532 17 Pardubice-Semtín, Czech Republic

Abstract:
Nowadays we are often confronted with limitation of quantity of explosives in terms of protection of surroundings, hygienic standards etc. Linear shaped charges (LSC) as such represent significant reduction in quantity of explosives (when compared with open charges) at blasting work, especially at demolitions of metal structures. Further decrease in quantity of explosives is achieved by tamping. This report deals with finding of relationship (represented by cavity depth produced by jet of LSC in steel plate with 30 mm thickness) between tamped and open LSC of the same performance.
NTREM, PARDUBICE, 2004 page 51-60

LIQUID PHASE AND SOLID PHASE NITRATION OF AROMATIC COMPOUNDS: GREEN SYNTHETIC ROUTES

D. Bahulayan*, C.P. Joshua and H.G. Ang***
* HEDM Research Laboratory, Faculty of Science, National University of Singapore, Science Drive 2, Singapore 117543
** Department of Chemistry, University of Kerala, Kariyavattom, Trivandrum, Kerala, India

Abstract

Selective mono- and di-nitration of aromatic hydrocarbons with various nitrating agents are discussed. Nitration of hindered diamines with potassium nitrate in conc. sulfuric acid yielded 80-95 % di-nitro derivatives. Nitration using 40% nitric acid with montmorillonite K10 and ferric nitrate supported on montmorillonite K10 showed high p-selectivity for mono-substituted substrates and also avoids the use of sulfuric acid. The total omission of sulfuric acid and the reduction of nitric acid concentration to 40% considerably reduce the emission of environmental pollutants. The montmorillonite K10 used as the solid support and catalyst is reusable by removing the water formed in the reaction followed by washing with acetone and subsequent drying in an air oven at 110 ºC.
NTREM, PARDUBICE, 2004 page 61-67

DEVELOPMENT OF ENERGETIC SALTS FOR PROPELLANTS

S. Beaucamp*, D. Mathieu* and V. Agafonov**
* Commissariat à l'Energie Atomique, Centre du Ripault, BP16, F-37260 Monts, France
** Laboratoire de Chimie Physique, EA PIMIR 2098, Faculté de Pharmacie, 31 Avenue Monge F-37200 Tours, France

Abstract:
The development of new energetic salt compounds composed by an ammonium cation fixed on an energetic nitrogen heterocycle and a nitrate anion are presented here. On one hand, these materials are more stable than their counterpart with nitro groups because of ionic charges which increase the cohesive energy. Despite the latter reduces the solid state heat of formation, the presence of ammonium and nitro groups on the energetic backbone decreases this effect. On the other hand, the nitrate group provides the oxygen necessary to generate stable reaction products. Moreover, the synthesis of these compounds requires methods to estimate their performances which depend on the density and the heat of formation. This provides information to lead chemists to promising components. A contribution groups method to estimate the density and semi-empirical methods to evaluate the heat of formation of salts have been developed because of the lack of suitable methods for ionic species.
NTREM, PARDUBICE, 2004 page 68-73

STUDIES ON THE NITRATION OF NEW POTENTIAL PRECURSORS FOR FOX-7

A.J. Bellamy*, N.V. Latypov and P. Goede****
* Cranfield University, Royal Military College of Science, Shrivenham, Swindon SN6 8LA, UK
**Swedish Defence Research Agency (FOI), SE-147 25 Tumba, Sweden

Abstract:
The initial microstructure of hot pressed polymer bonded explosives and its evolution under thermal and mechanical aggressions were studied. The thermal aggressions include low temperature freezing and frozen combustion. Mechanical aggressions include tension, compression, ultrasonic wave insult and long-pulse low-velocity impact. The mechanical properties under tension and compression were studied and compared. Brazilian test was used to study the tensile properties. The failure mechanisms of polymer bonded explosives under different loading conditions were analyzed.
NTREM, PARDUBICE, 2004 page 74-81

A 1:1 HNS-DIOXAN COMPLEX

A.J. Bellamy and T.P. Price
Department of Environmental and Ordnance Systems, Cranfield University, Royal Military College of Science, Shrivenham, Swindon SN6 8LA, UK

Abstract:

HNS IV is commonly produced by crash precipitation of a DMF or NMP solution into water. The product usually contains 0.5-1.5 wt% of solvent trapped inside the HNS crystals. This residual solvent may be removed by washing with methanol containing dioxan. However this also causes a dramatic change in particle shape and size, and, unless further washed with pure methanol, the product will contain a considerable amount of dioxan. We have found that this dioxan-containing HNS is in fact a 1:1 complex with a different crystal structure to that of pure HNS. The dioxan may be removed from the complex by either heating above the boiling point of dioxan or washing with methanol. This does not significantly change the outward appearance of the crystals, but it does change the inner structure to that of normal HNS.

NTREM, PARDUBICE, 2004 page 82-88

DETERMINATION OF RESIDUE OF EXPLOSIVES IN ENVIRONMENTAL SAMPLES

J. Błądek, S. Pietrasiak and S. Cudziło

Institute of Chemistry, Military University of Technology, Kaliskiego 2, 00–908 Warsaw, PL

Abstract:

Modern TLC equipment was used for determination of 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX, hexogen) post-detonation residues in environmental samples. Chromatographic system suitable for the analyte separation from matrix components and method of densitometric determination of RDX was proposed. A linear dependence of densitometric peak areas A on the analyte mass c [ng] in the chromatographic band was received (A = 26.302 -c - 484). A limit detection (150 ng) and maximal range of linear measurements (1800 ng) were determined. Methods of extraction were specified and recoveries of RDX were estimated (they were about 70%).

NTREM, PARDUBICE, 2004 page 89-93

CHARACTERIZATION OF THE CARBONACEOUS PRODUCTS OF HALOGENOCARBONS REDUCTION IN COMBUSTION WAVE

S. Cudziło*, W. Kiciński*, J. Błądek*, A. Arciszewska* and A. Huczko**

* Institute of Chemistry, Military University of Technology, Kaliskiego 2, 00–908 Warsaw, PL

** Department of Chemistry, Warsaw University, Pasteura 1, 02-093,Warsaw, PL

Abstract:

In the paper a method of synthesis of carbonaceous materials in self-propagating heat waves is described and results of some physical and chemical investigations of the materials are presented. The chemical (ultimate analysis) and phase (XRD) composition as well as the microstructure (SEM) of the solid reaction products were determined. Next the relation between reactant composition and heats of reaction as well as the amount, type and structure of the reaction products was established. It was shown that some of the obtained materials are characterized by unique structural and surface properties.

NTREM, PARDUBICE, 2004 page 94-99

STUDY ON COMBUSTION OF LIQUID AND GELATINIZED GLYCIDYL AZIDE OLIGOMERS

V.Y. Egorshev, V.P. Sinditskii and M.V. Berezin

Mendeleev University of Chemical Technology 9 Miusskaya Square, 125047, Moscow, Russia

Abstract

Effect of the molecular weight ofglycidyl azide oligomers on the burning rate and effect of gelatinization have been examined. It has been shown that combustion of uncured GAP obeys usual rules of monopropellant burning of liquid energetic materials with all resulting consequences (turbulization, unusual burn rate-pressure dependence, etc.). Small additives ofPMMA, used as a

gelatinizing agent to GAP oligomers appeared to influence drastically their burning behavior through alteration of the viscosity. Data on combustion of uncured neat azide oligomers and their compositions with the polymer as well as data of temperature measurements in the combustion wave have been used to propose the combustion mechanism of azide energetic materials.
NTREM, PARDUBICE, 2004 page 100-114

INVESTIGATION OF DIAMINODINITROETHYLENE (DADNE)

N.V. Garmasheva, I.V. Chemagina, V.P. Filin, M.B. Kazakova and B.G. Loboiko
Zababakhin Russian Federal Nuclear Centre - VNIITF, P.O. Box 245, Snezhinsk, Chelyabinsk region, 456770, Russia

Abstract:
DADNE (FOX-7 or 1,1-diamine-2,2-dinitroethylene) is investigated by methods of differential-thermal (DTA) and thermo-gravimetric (TGA) analyses. Two exothermal peaks that, presumably, correspond to transitions between polymorphic modifications of this HE, are registered on DTA curve. Heat of low-temperature polymorphic transition (~±113°C) is estimated as ~ 25 J/g. Heat of high-temperature transition (~+158°C) is ~20J/g. Presence of two exothermic peaks (+207ºC and +277ºC under the heating rate of 2ºC /min) on DTA of DADNE is confirmed. It is shown, that DADNE decomposes in two stages at heating over +210ºC . The product of the first stage of decomposition of DADNE is new explosive (DADNE-T). The DTA, TGA, FTIR ofDADNE-T are carried. The endothermic processes in DADNE-T in the temperature range +20 °C - 400 °C are not founded. The beginning of exothermic decomposition of DADNE-T is recorded. By results of FTIR it is supposed that DADNE-T is the product of chemical transformation of two molecules of DADNE with participation of the part of amino and nitro groups. The crystals of three types (tetrahedral prisms, crystals of the trimetric form and hexahedral prisms) are received at crystallization of DADNE from acetone, water and water-acetone mixes. Received crystals are investigated by methods of FTIR, DTA and TGA.
NTREM, PARDUBICE, 2004 page 115-121

ESTIMATION OF THE THERMODYNAMIC PROPERTIES OF SOLID PROPELLANTS

S. Gheorghian
Academia Tehnică Militară, George Coşbuc bd. nr. 81-83, 050141 Bucureşti, România

Abstract:
The paper presents a theoretical method, based on Corner's method, for the estimation of the thermodynamic properties of solid propellants. The mathematical model contains the truncated virial equation of state, the equilibrium constant equation for each chemical reaction, the mass and energy conservation equations. The virial coefficients were calculated from the intermolecular forces using the Lennard-Jones 6,12 potential function. Based on this model, a computer program, called REAL, has been written. At the end, one presents some results obtained with this program for three gun propellants.
NTREM, PARDUBICE, 2004 page 122-131

APPLICATION OF NOVEL ENERGETIC MATERIALS FOR INITIATORS AND EXPLOSIVE TRAINS

J. Hamid, T. Griffiths, R. Claridge and T. Jordan
QinetiQ Ltd., Energetic Materials Dept., MOD Fort Halstead, Sevenoaks, Kent, UK

Abstract:
As well as improving the survivability of weapons and platforms, Insensitive Munitions (IM) reduce both casualty rates and mission losses. Their use also leads to improved safety during storage and transportation. For a munition to completely fulfil IM criteria each of its energetic sub-systems must be IM compliant.

The initiator and explosive train are the most critical of these sub-systems; their safety and reliability are paramount if the weapon is to be suitable for service use. They are generally the most difficult part of a weapon system to protect from inadvertent initiation since their primary function is initiation of the main charge explosive. In the last decade, a number of new high temperature compounds with improved power outputs and potential for both exploding foil initiator (EFI) and explosive train applications have been reported. Several of the more promising materials based on pyrazine, pyridine and polynitro- aromatic systems have been successfully synthesised and characterised.

NTREM, PARDUBICE, 2004 page 132-140

MICROSTRUCTURE, MECHANICAL PROPERTIES AND MECHANICAL FAILURE OF POLYMER BONDED EXPLOSIVES

Peng-wan CHEN*, Feng-lei HUANG*, Yan-sheng DING**

* National Key Laboratory of Explosion and Safety Science, Beijing Institute of Technology, Beijing 100081, China

** Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China

Abstract:

The initial microstructure of hot pressed polymer bonded explosives and its evolution under thermal and mechanical aggressions were studied. The thermal aggressions include low temperature freezing and frozen combustion. Mechanical aggressions include tension, compression, ultrasonic wave insult and long-pulse low-velocity impact. The mechanical properties under tension and compression were studied and compared. Brazilian test was used to study the tensile properties. The failure mechanisms of polymer bonded explosives under different loading conditions were analyzed.

NTREM, PARDUBICE, 2004 page 141-148

SYNTHESIS AND CHARACTERISATION OF NITROGUANIDINE BASED NITRATE AND PERCHLORATE SALTS OF-5-NITRO-2-NITROIMINOHEXAHYDRO-1,3,5-TRIAZINE

H. S. Jadhav*, M. B. Talawar*, D. D. Dhavale*, S. N. Asthana*** and V. N. Krishnamurthy****

* Department of Chemistry, Garware Research Centre, University of Pune, Pune 411007, INDIA

** DRDO/ISRO Cell, University of Pune, Pune 411 007, INDIA

*** High Energy Material Research Laboratory, Sutarwadi Pashan, Pune 411 021, INDIA

Abstract:

The condensation of nitroguanidine, formaldehyde and amine followed by nitration afforded 5-nitro-2-nitroiminohexahxdro-1,3,5-triazine (2). Compound 2 on nitric acid and perchloric acid treatment afforded the nitrate and perchlorate salts of 2.

NTREM, PARDUBICE, 2004 page 149-156

DETERMINATION OF LOW CONCENTRATION TRINITROTOLUENE CONTENT IN WATER SAMPLES

V. Ježová*, J. Skládal, A. Eisner*, L. Gollová* and K. Ventura ***

* Department of Analytical Chemistry, University of Pardubice, 53210, Pardubice, Czech Republic

** Research Institute of Industrial Chemistry, Explosia a.s., 53217, Pardubice - Semtín, Czech Republic

Abstract

Polynitroaromatic organic explosives (2,4,6-trinitrotoluene) are typical labile and environmental

that can transform with soil indigenous microorganisms, photodegrade by sunlight and migrate though subsurface soil to cause groundwater contamination. To be able to determine the type and concentration of explosives and their (bio)transformation products in different soil environments, a comprehensive analytical methodology of sample preparation, separation and detection in thus required. This present paper describes the use of solid-phase microextraction (SPME) and solid-phase extraction (SPE) for the extraction of nitroaromatic explosives for subsequent analysis by either GC/MS or HPLC/UV. The two techniques are examined in terms of procedure, chromatographic analysis and method performance.
The adsorption temperature and adsorption times were examined by the using SPME fiber. SPE extraction was done by variable columns and microcolumns and was examined the columns with high efficiency and with short sorption time.
NTREM, PARDUBICE, 2004 page 157-163

SENSITIVITIES AND PERFORMANCES OF NON-REGULAR EXPLOSIVES

M.H. Lefebvre, B. Falmagne and B. Smedts
Laboratory of Energetic Materials, Royal Military Academy, Brussels - Belgium

Abstract:
Some chemical characteristics, safety properties and explosive performances of two explosives are investigated, namely tri-aceton-tri-peroxide (TATP) and hexa-methyl-triperoxyde-diamine (HMTD). Production is relatively easy to perform with quite easily available materials, but the purity, the quality and the properties of the explosive crystals are quite dependent on the synthesis process. Pure and unpurified compounds are tested for both their sensitivities and performances. The sensitivity to friction and to impact is determined and compared with values of other energetic materials. The performances of small explosive charges (up to a few grams) are evaluated: brisance and initiation capability. The detonability and brisance of the compounds are observed and characterized using standard aluminum witness plates. The study shows that TATP can be used efficiently - at own and great risk of the technician - as secondary as well as primary explosive, accounting for a good versatility of the compound.
This work shows the great risks associated with these two peroxides but also why some of their characteristics make these explosives popular among certain groups.
NTREM, PARDUBICE, 2004 page 164-173

RESEARCH ON THE INFLUENCE OF AMMONIUM NITRATE PRILL PROPERTIES ON DETONATION PARAMETERS OF ANFO AND THEIR MIXTURES WITH DOUBLE BASE PROPELLANTS

K. Lipińska*, M. Lipiński*, A. Maranda and J. Sobala*****
* Institute of Industrial Organic Chemistry, 6 Annopol St., 03-236 Warszawa, Poland
** Military University of Technology, 2 Kaliskiego St., 00-908 Warszawa, Poland
*** Central Mining Institute, 1 Gwarków Sq., Katowice, Poland

Abstract:
Properties of ammonium nitrate prills determine the physical stability and detonation characteristics of ANFO. Some physical characteristics of ammonium nitrate prills (apparent density, specific surface area and structure examinations by scanning electron microscopy) were determined. We investigated the influence of commercial ammonium nitrate prill properties on detonation velocities of some explosives. They included commercial ANFO explosives and their mixtures with demilitarized double base propellants of different nitroglycerine content. Results suggest that double base rocket propellants can increase detonation parameters of mining explosives.
NTREM, PARDUBICE, 2004 page 174-182

BEYOND THE GROUP CONTRIBUTION APPROACH TO

FLUID PROPERTIES: NEW MODELS FOR THE DENSITY AND THERMAL STABILITY OF ENERGETIC COMPOUNDS

D. Mathieu, J.-P. Becker and E. Theerlynck
Commissariat à l'Energie Atomique, Centre d'Etudes du Ripault, BP 16, 37260 Monts, France

Abstract:
Many properties of molecular fluids may only be estimated using group contribution methods. Some of them lend themselves naturally to such an additive scheme (e.g. the density) while this is not the case for others (e.g. the thermal stability). Alternative models are presented to calculate the density and decomposition temperature of molecular liquids. For the density, the accuracy of the new scheme is similar to that of the most reliable available methods, despite a drastic reduction of the number of empirical parameters. For thermal stability, a simple kinetic model is shown to be a better basis to develop predictive tools than any group contribution schemes.
NTREM, PARDUBICE, 2004 page 183-189

IDENTIFICATION OF SOLID PROPELLANT COMBUSTION DYNAMIC CHARACTERISTICS FROM THE RESULTS OF EXPERIMENTS WITH REGISTRATION OF THE CURRENT BURNING FRONT POSITION

Y.M. Milyokhin*, A.N. Klyuchnikov*, A. V. Fedorychev*, S.V. Gunin*, V.V. Serushkin, V.P. Sinditskii ** and S.A. Filatov ****
* Federal Center of Dual-Use Technologies "Soyuz", Academician Zhukov St. 42, 140090, Dzerzhinsky, Moscow region, Russia
** Mendeleev University of Chemical Technology, 9 Miusskaya Square, 125047 Moscow, Russia

Abstract:
A stable algorithm of structural and parametric identification of combustion dynamic characteristics from the results of experiments with registration of the current burning front position has been developed, which allows prediction of current values of burning rate $U(T)$ and its frequency response with accuracy acceptable to practice. The proposed approach has been tested by simulation calculations with harmonic input signals, including superimposed noise of different intensity, to determine the accuracy of identification of the amplitude and phase frequency characteristics of burning. The approach has been used to study dynamic combustion characteristics of a model propellant under oscillating pressure. The transfer and response functions have been determined for a low frequency area. It has been shown that the approach is favorably distinguished from other procedures by higher accuracy and authenticity of estimations.
NTREM, PARDUBICE, 2004 page 190-201

DEVELOPMENT OF COMPUTER CODE FOR QUALITATIVE PREDICTION OF HEAT OF FORMATION OF HIGH ENERGETIC MATERIALS

Part I

H. Muthurajan*, R. Sivabalan, M.B. Talawar** and S.N. Asthana****
* Armament Research and Development Establishment, Pashan, Pune-411021, India ** High Energy Materials Research Laboratory, Sutarwadi, Pune-411 021, India

Abstract
A computer code has been developed to predict heat of formation based on two methodologies. In first methodology, the logic ofStine and Kramer method of predicting heat of formation has been used and extended to terminal functional groups such as -OH, -NH, -NH_2, -NO2, -H and C=O. In the second methodology, a new equation for heat of formation has been derived by merging the equations of Stine et al and Rothsetien et al, which are being used for the theoretical prediction of velocity of detonation. The linear regression coefficient R^2 = 0.9387 and 0.8358 are obtained for

heat of formation predicted by this code and compared with those reported in literature, using methodology I and II respectively This new technique of predicting heat of formation from elemental composition ofHEM's has been successfully appended in a windows based user-friendly software code named LOTUSES (Linear Output Thermodynamic User-friendly Software for Energetic Systems) developed by our team. The LOTUSES code also simultaneously predicts properties such as molecular weight, oxygen balance, velocity of detonation, C-Jpressure, density, heat of explosion, relative strength of an explosive in comparison to 2,4,6-trinitro toluene (TNT) as well as the possible explosive decomposition products after explosion, volume of explosion products and air blast effects has been reported recently by authors. The predicted heat of formation by LOTUSES can be stored in various formats such as .txt, .html, .doc, .pdf and can be saved either in hard disk or even in floppy diskettes/compact diskette. The predicted output can also be copied into RAM, which can be pasted in other softwares such as microsoft word/powerpoint etc.,. Also output of the predicted heat of formation can be heard/listen from speakers attached to the PC through multimedia sound card.

NTREM, PARDUBICE, 2004 page 202-223

STUDY OF TNT METABOLISM IN PLANTS AND ITS PRACTICAL APPLICATION FOR ENVIRONMENT DECONTAMINATION

A. Nepovím*, R. Podlipná*, S. Zeman, Z. Jalový**, A. Gerth*** and T. Vaněk***

* Institute of Organic Chemistry and Biochemistry, Flemingovo nám. 2, CZ-166 10 Praha 6

** DTTX, University of Pardubice, CZ-532 10 Pardubice

***Bioplanta GmbH, Benndorfer Landstraße 2, D-04509 Leipzig

Abstract:

Although a contamination of sites by TNT is an environmental problem all over the world, the fate of its degradation products claims attention as well. A study of metabolism of TNT in plants was focused on degradation of 4-amino-2,6-dinitrotoluene (4-ADNT), a stable degradation product. Two plant species Senecio jacobea and Buphthalmum salicifolium cultivated under in vitro conditions in the presence of different concentration of 4-ADNT for 3 weeks. The highest concentration 50 mg/l of 4-ADNTwas degraded by plants within two weeks but any major degradation product was not detected in the medium. The IC_{50} was not determined in the range of used concentration therefore a linear regression was used for prediction of the IC50 and 61,8 mg/l and 70,2 mg/l were calculated for S. jacobea andB. salicifolium, respectively.

NTREM, PARDUBICE, 2004 page 224-226

TEMCLEV-EX. ADAPTATION OF TEMCLEV SYSTEM TO FIRE AND EXPLOSION HAZARD ASSESSMENT IN MANUFACTURING OF EXPLOSIVES

T. Piotrowski, T. Sałaciński, M. Frączak and D. Buczkowski

Instytut Przemysłu Organicznego, Annopol 6, 03-236 Warszawa, Poland

Abstract:

The main assumptions of a new research-technical project have been presented, which aim is to adapt the system of evaluation and classification the process hazards in chemical industry, called shortly Temclev, to the specificity of manufacturing of explosives. A brief description of the original Temclev system has been given as well as a direction of its transformation into a new version - Temclev-Ex.

NTREM, PARDUBICE, 2004 page 227-233

EXPERIMENTAL INVESTIGATION OF IGNITION MECHANISMS IN CONFINED ENERGETICS

H. J. Prentice and W. G. Proud
Cavendish Laboratory, University of Cambridge, Cambridge, UK

Abstract:
Detailed understanding of the response of confined energetic materials to different stimuli is critical to their design. This paper presents an experimental investigation of ignition mechanisms in Detasheet (a polymer-bonded explosive) when confined between copper plates and impacted at normal incidence with copper plates at velocities up to 600 m/s. High-speed photography and optical fibres are used to detect points of ignition and consequent reaction history. PVDF stress gauges are used to relate velocity of impact with pressure generated in the explosive A Hugoniot curve for detasheet has been plotted.
NTREM, PARDUBICE, 2004 page 234-242

THE ETHICS OF ANALYSIS AND MEASUREMENT IS YOUR ANSWER THE CORRECT ANSWER?

Fritz van Rooyen
National Institute for Explosives Technology (NIXT) South Africa PO Box 32544, Glenstantia 0010, Pretoria. Republic of South Africa

Abstract:
In spite of careful analysis and measurement, results are often incorrectly calculated and reported. This may have serious effects on the outcomes of the investigation -products, ammunition and associated systems may not meet the specifications and miss the target, time and materials are wasted and revenue eventually lost. This paper deals with the necessity for and principles of correct scientific numerical communication. The basic measuring units are initially reviewed followed by a discussion of the proper use of figures and correct handling of measurements. In conclusion the nature of measuring errors is studied and guidelines for its prevention provided. A number of exercises are provided in the text, the answers to be found at the end of the paper. The ultimate aim will be to improve the reliability of the reader as an analyst/researcher.
NTREM, PARDUBICE, 2004 page 243-261

THERMAL AND THERMO-MECHANICAL INVESTIGATIONS OF LONG TIME STOREDPROPELLANTS

P. Shishkov, T. Tzvetkoff, I. Glavchev and R. Ganev
University of Chemical Technology and Metallurgy, 8. Ohridski Str. Kl., 1756 Sofia, Bulgaria

Abstract:
Samples of single based propellant (SBP) and double based propellants (DBP) stored a long time in non-heated military store houses were investigated up to 393 K. The dependences temperature / deformation were made by the heating rate 2oC/min. and the values of glass transition temperature (Tg) were determined. With the Flory-Fox-Biky equation the values of Tg(∞) and K were calculated. After measuring the dimensions of the samples in several temperatures were calculated the coefficient of thermal expansion of the propellants. The influence of the time of storage of the propellants on their properties was determined.
NTREM, PARDUBICE, 2004 page 262-267

INFLUENCE OF VELOCITY OF GAS FLUX TO THE BURNING SURFACE

M. Šimáček*, V. Kuttelwascher* and P. Stojan**
* Military Academy in Brno, Faculty of Airforces and Air Defence, Kounicova 65, CZ-602 00, Brno, Czech Republic

** Explosia a.s., Research Institute for Industrial Chemistry, CZ-532 17, Pardubice - Semtín, Czech Republic

Abstract:
This paper includes the solution of testing Solid Propellant Rocket Motor with erosive burning part of burning process when gas generator is used for the purpose mentioned. Students of doctor's study programs of Military Academy in Brno and members of Explosia a.s. provided the realisation of these tests.
NTREM, PARDUBICE, 2004 page 268-275

HIGH RESOLUTION OPTICAL ANALYSIS OF DYNAMIC EXPERIMENTS ON PBXs

C.R. Siviour, S.G. Grantham, D.M. Williamson, W.G. Proud, S.M. Walley and J.E. Field
PCS Group, Cavendish Laboratory, Cambridge, CB3 0HE, United Kingdom

Abstract:
Previous research [m] has provided information on the high strain rate behaviour of energetic systems. This paper outlines developments in the measurement of strain fields and strain localisation. In particular, the conditions for strain localisation in materials are discussed. The application of a photographic technique, digital speckle metrology, allows deformation fields to be measured. Although this does not provide sufficient resolution for strain localisations to be observed in detail, this aspect is being actively pursued.
NTREM, PARDUBICE, 2004 page 276-283

INFLUENCE OF NC PROPELLANT SAMPLE SELF-HEATING ON ARRHENIUS KINETIC CONSTANTS DERIVED FROM NON-ISOTHERMAL DSC MEASUREMENTS

M. Sućeska, S. Matečić Mušanić and M. Rajić Linarić
Brodarski Institute, Av. V. Holjevca 20, 10000 Zagreb, Croatia

Abstract:
Non-isothermal isoconversional kinetic methods described by Ozawa, and Flynn and Wall are widely used to study kinetics of energetic materials. However, to obtain valuable kinetic constants great care must be taken to ensure proper experimental conditions, as well as data treatment procedure.
In this paper we have discussed the influence ofNCpropellant sample mass and heating rate during non-isothermal DSC measurements, i.e. the influence of NC propellant sample self-heating on kinetic results derived in accordance with the Ozawa and Flynn and Wall methods.
It was calculated by the Ozawa method that the activation energy equals ~199 kJ/mol in the case when sample self-heating has been avoided, while in the case of sample self-heating existence the activation energy was calculated to be ~191 kJ/mol. Also, it was shown that the activation energy calculated by the Flynn and Wall method depend not only on sample self-heating existence but also on degree of conversion - it ranges between ~145 and 200 kJ/mol.
NTREM, PARDUBICE, 2004 page 284-297

MECHANICAL PROPERTIES OF GEL-PROPELLANTS WITH NANOPARTICLES

U. Teipel, U. Förter-Barth and H. Krause
Fraunhofer Institute for Chemical Technology (ICT), P.O. Box 1240, 76318 Pfinztal, Germany

Abstract:
Gel propellants provide rocket propulsion systems of high specific impulse, low sensitivity and low vulnerability in combination with the capability to control the thrust, i.e., variation of thrust and thrust cut off. The rheological characterization is essential for the development of adequate gel

propellant formulations and thus for the design of an applicable propulsion system. In this contribution, the rheological behavior of a gel propellant consisting of nitromethane as fuel and nanoparticles of silicon dioxide as gelling agent was examined. The experiments were conducted under steady state shear flow and oscillatory shear. The nitromethane/silicon dioxide gels exhibit non-Newtonian flow behavior over the whole concentration range examined. Additionally, a yield stress is determined for all the gels. The viscoelastic properties are typically gel-like in that the storage and the loss moduli are both independent of frequency.
NTREM, PARDUBICE, 2004 page 298-305

STUDY OF SUB-MICRON STRUCTURED PHOTOSENSITIVE PRIMARY EXPLOSIVES FOR LASER INITIATION SYSTEMS

I.A. Ugryumov, M.A. Ilyushin, I.V. Tselinsky, A.S. Kozlov, V.Yu. Dolmatov, I.V. Shugalei and A.N. Golovchak

St.-Petersburg State Institute of Technology (Technical University), 190013, St.-Petersburg, Russia

Abstract:

Synthesis of nano-structures with predetermined characteristics and development of functional materials on their basis have become one of the priority problems in the materials science. Nano-particles possessing the size in the range 1-100 nanometers often show in comparison with materials formed by particles of the micron size often possess unusual characteristics . Working out energetic condensed systems, especially photosensitive primary explosives for the systems of laser initiation is one of the primary branches of application of nano-structured materials. We have synthesized and investigated mercury (II) complex perchlorate with 5-hydrazinotetrazole as a ligand (compound (I)) as a potential photosensitive primary explosive. This complex having particles of 1.1 ±0.8 μm size demonstrated the highest sensitivity to laser irradiation combined with an extremely low initiation threshold. On the basis of compound (I) the photosensitive formulation EC-2 containing ~ 90 % of the complex mercury perchlorate and ~ 10 % of an optically transparent polymer as an inert matrix has been proposed. Formulation EC-2 has externally high sensitivity to Q-switch IR-laser irradiation. Formulation EC-2 with added ultra disperse diamonds (UDD) (<100 nm) has shown lower initiation thresholds in comparison with neat EC-2 or EC-2 with added sub-micron black carbon instead of UDD. To increase the safety, an optical detonator on the basis of EC-2 separated from the high explosive charge (HE) by a metal cup, has also been studied.
NTREM, PARDUBICE, 2004 page 306-316

STUDIES AND RESEARCHES REGARDING THE UTILIZING OF RESULTS OBTAINED AT THE BURNING OF POWDER IN CLOSE BOMB FOR SOLVING OF FUNDAMENTAL PROBLEM OF INTERIOR BALLISTICS

T. Vasile, C. Barbu and D. Safta

Military Technical Academy, 81-83 George Cosbuc Avenue, Bucharest, Romania

Abstract:

In this paper it is presented a mathematical model of firing phenomenon, using the results obtained during of the powder burning in close bomb. On the base of the mathematical model was elaborated an interior ballistic soft, which allows to study the variation of the powder gases pressure and the projectile velocity versus its displacement inside of grooved barrel and versus time. For an extant weapon, the theoretical results that was obtained with the aid of this soft and the experimental data are compared.
NTREM, PARDUBICE, 2004 page 317-324

EFFECTS OF THE COATING PROCESS OF HE MOULDING POWDERS ON SAFETY AND IM CHARACTERISTICS

R. Wild
PBX-Center Maasberg, Diehl Munitionssysteme GmbH & Co KG, Karl-Diehl-Straße 1, D-66620 Nonnweiler, Germany

Abstract:
High performance warheads are very demanding on every component of the whole system. The HE "low cost" component has to fulfil performance and IM criteria. Two coating methods, slurry and paste process, promise better results and effectiveness for new moulding powders.
NTREM, PARDUBICE, 2004 page 325-332

BALLISTICAL AND CHEMICAL STABILITY OF ROLLED BALL PROPELLANTS

S. Wilker*, P. Guillaume, M.H. Lefebvre***, S. Chevalier**** and Laurence Jeunieau*****
* WIWEB ASt Heimerzheim, Großes Cent, 53913 Swisttal (DE)
** PB Clermont S.A., Rue de Clermont 176,4480 Engis (BE)
*** Ecole Royale Militaire, Avenue de la Renaissance 30,1000 Bruxelles (BE)
**** SME - Centre de Recherches Le Bouchet, Boîte Postale Nº2, 91710 Vert-le-Petit (FR)

Abstract
This paper presents in summary the work of a Belgian-French-German cooperation programme on the chemical and ballistical stability of a ball propellant for the 5.56 · 45 mm ammunition. The programme comprises thermoanalytical, analytical, ballistical and spectroscopical techniques applied on unaged and aged samples of the propellant K 5810.
The propellant K 5810 is chemically stable. This fact is proven by microcalorimetry; the maximum heat flow does not reach the limit values of STANAG 4582. Also the stabilizer content after ageing times which are comparable to a 10 years storage at 25°C is much higher than the limit values given in AOP-48, Ed. 2. The ageing mechanism is strongly dependent on the loading density of the ampoules and the atmosphere above the sample which underlines the big effect oxygen has on the ageing of nitrocellulose based propellants.
The slight energy loss during the ageing periods used here does not affect the ballistic behaviour significantly. In contrast to the 9 mm ammunition tested before there seems to be no incompatibility between the propellant and the Sintox primer because the propellant K 5810 does not contain isopropanol in contrast to the K 6210 propellant in the 9 mm ammunition.
The ballistic life time is limited by the migration of the deterrent. This migration leads to an increased burning rate and thus to an increased pressure in the early phase of the burning reaction. As not all samples are available at the moment a final value for the activation energy of the migration of the DBP can not be given. First estimations lead to a value slightly above the activation energy of the nitrate ester decomposition.
NTREM, PARDUBICE, 2004 page 333-347

DEFORMATION AND FRACTURE OF ENERGETIC MATERIALS AND THEIR SIMULANTS

D. Williamson, S. Palmer, J. Field and W. Proud
University of Cambridge, Cavendish Laboratory, Physics and Chemistry of Solids Group, Madingley Road, Cambridge, CB3 0HE, United Kingdom

Abstract:
A detailed understanding of the deformation and fracture mechanisms of energetic materials is vital to ensure optimum performance and safety. A series of deformation and fracture experiments with optically derived results are being developed on a sugar based energetic simulant with the ultimate aim of transferring the proven experiments to energetic materials. The physical insight and quantitative data these experiments yield are crucial in developing accurate and predictive models of the response of energetic materials to mechanical stimuli. This paper outlines the results taken to

date and future research
NTREM, PARDUBICE, 2004 page 348-358

ON THE REACTIONS OF 2-(DINITROMETHYLENE) -4,5-IMIDAZOLIDINEDIONE WITH ALKALINE AGENTS

Shu Yuanjie, Cai Huaqiang, Huanghui and Cheng Bibo
Institute of Chemical Materials CAEP, 621900, Mianyang, Sichuan, China

Abstract:
The new preparation methods of 1,1-diamino-2,2-dinitroethylene and 2-dinitromethylene-4,5-imidazolidinedinefrom 2-methylimidazole were studied. The yield of2-dinitromethylene-4,5-imidazolidinedione was 20.3% by nitrating 2-methylimidazole in the sulfuric and nitric acid. Under different alkaline conditions, 2-dinitromethylene-4,5-imidazolidinedione can process two different reactions: in the alkalescent conditions, the main product is Fox-7; with alkali conditions, the main product is potassium dinitromethanate. By optimizing reaction conditions, the yield of Fox-7 could be up to 95.3% and for potassium dinitromethanate, it coulde be 65%.
NTREM, PARDUBICE, 2004 page 359-364

MECHANISTIC STUDIES OF DESTRUCTIVE NITRATION OF 2-ALKYL SUBSTITUTED 4,6-DIHYDROXY PYRIMIDINES

A. A. Astratev, D.V. Dashko, A. I. Mershin and A. I. Stepanov
Special Design and Construction Bureau SDCB "Technolog " of the Saint-Petersburg State Institute of Technology 190013,, Saint-Petersburg, Moskovskiypr.26; Russia

Abstract:
The main stages of destructive nitration of 2-(4-oxo-6-hydroxy-2-pyrimidinylidene) acetic acid in various nitrating mixtures have been identified. The effect of consecutive introduction ofnitro groups on the formation of the key intermediate responsible for the generation of 1,1-diamino- 2,2-dinitroethylene (DADNE, FOX-7) has been demonstrated. A general scheme of chemical transformations of 2- methyl-4, 6-dihydroxypyrimidine under the conditions of acidic nitration has been suggested.
NTREM, PARDUBICE, 2004 page 365-372

SIMULATION STUDY ON ARMOUR-PIERCING EFFECT OF ARMOUR-PIERCING BOMB

Zhou Renbin*, Xie Tiebang* and Xiang Weixiang**
* Huazhong University of Science and Technology, School of Mechanical Science and Engineering, Wuhan, Hubei, 430074, P.R.China
** Wuhan Ordnance Noncommissioned Officer Academy of PLA, Department of artillery, Wuhan, Hubei, 430075, P.R.China

Abstract:
Studying the armor-piercing effect of Armour-piercing bomb that attacks aluminum target is essential because the target can be considered the simulation of the actual fight equipment. Based on the hypothesis about building the fraction field, the armor-piercing effect of armor-piercing bomb is analyzed, and the velocity and the intruding depth parameter model of armor-piercing effect are established. Taking a certain armor-piercing bomb as example, the intruding processes of armor-piercing effect are simulated by using the nonlinear finite element analysis program LS-DYNA, while aluminum target simulates the wall of combat equipment in two different conditions. At last, the finite element simulated results are given and analyzed that agree with the experiments.
NTREM, PARDUBICE, 2004 page 373-379

EFFECT OF TNT CHARGES ORIENTATION ON GENERATED AIR BLAST WAVES NUMERICAL SIMULATION USING LS-DYNA

V. Adamík*, J. Vágenknecht, P. Vávra** and W.A. Trzciński*****

* External Consultant of the DTTX on Continuum Dynamics

** Department of Theory and Technology of Explosives University of Pardubice, 532 10 Pardubice, Czech Republic

*** Military University of Technology, Kaliskiego 2, 00 980 Warsaw, Poland

Abstract

The paper deals with numerical 3D simulation, through the code LS-DYNA, of the effects caused by air blast waves generated by cylindrical TNT charges (the mass of25g and 50g) which are differently oriented respect to the pressure gauges placed relatively close to the charges (approximately 800 mm and 840 mm from the charges). As the first step for these simulations, the numerical study has been concentrated on the verification of the state equations for TNT and air continuum. It has been concluded that the JWL equation of state and ideal gas equation of state were proper representations for TNT and air respectively. Then, simple formulae for various oriented charges have been developed and verified. These formulae make possible to represent the original cylindrical charges like equivalent 3D ellipsoids (this approach is very important in order to obtain stable computational mesh). The final numerical simulations have been compared with the original experiments performed at Military University of Technology in Warsaw. On the base of this comparison, it has been concluded that the 3D numerical simulations using LS-DYNA have been a very powerful and useful tools.

NTREM, PARDUBICE, 2004 page 380-389

DETERMINATION OF THE CONSEQUENCES OF POSSIBLE INDUSTRIAL ACCIDENTS

V. Adamík*, B. Janovský and A. Tkáč*****

* External Consultant of the DTTX on Continuum Dynamics, CZ

** Department of Theory and Technology of Explosives, University of Pardubice, 532 10 Pardubice, Czech Republic

*** Nuclear Power Plants Research Institute, Okružná 5, 918 64 Trnava, Slovak Republic

Abstract:

The paper is devoted to calculations of the consequences relating to accidental vapour cloud explosions. For this purpose, a general methodology has been developed and applied. The methodology consists of two steps: the first one deals with blast wave characterization - Multi-Energy method has been used, the second one deals with the propagation of the generated blast wave in surrounding air and wave-building interaction - the LS-DYNA code has been applied. The methodology has been applied to a case ofunconfined non-obstructed hydrogen cloud explosion in site. An example of the application is presented in the paper. The methodology presented can be used both to determine the consequences of an accidental vapour cloud explosions for risk analysis purpose and at the same time also as an optimalization design tool which enables to minimize consequences of possible explosions taking into account various plant layouts.

NTREM, PARDUBICE, 2004 page 390-400

TOPOGRAPHY OF REACTION ORIGINATION OF SILVER AZIDE EXPLOSION DECOMPOSITION UNDER INITIATION BY ELECTRON ACCELERATOR PULSE[1]

B.P. Aduev*, V.P. Filin, E.V. Tupitsin*, G.M. Belokurov*, D.E. Aluker* and A.S. Pashpekin***

* Kemerovo State University, 650043, Kemerovo, Russia,

** Russian Federal Nuclear Center, All-Russia Research Institute of Technical Physics (RFNC-VNIITF) 456770, PO Box 245, Snezhinsk, Chelyabinsk region, Russia

Abstract:
The silver azide pre-explosive luminescence origination by electron pulse initiation in nidi and subsequent broadening of the luminescence ranges overlapping finally the whole sample. Hence, the origination nidi of the reaction are not caused by the local heating and they are not the hot spots in the true sense of the word.
NTREM, PARDUBICE, 2004 page 401-403

SPECTRAL-KINETIC CHARACTERISTIC OF PETN LUMINESCENCE UNDER INITIATION BY ELECTRON BEAM[1]

B.P. Aduev*, G.M. Belokurov*, N.V. Garmasheva, S.S. Grechin*, E.V. Tupitsin*, and V.N. Shvayko****

* Kemerovo State University, 650043, Kemerovo, Russia
** Russian Federal Nuclear Center, All-Russia Research Institute of Technical Physics (RFNC-VNIITF) 456770, PO Box 245, Snezhinsk, Chelyabinsk region, Russia

Abstract:
Spectral-kinetic characteristics of PETN single crystal explosive luminescence under initiation by a high-strength electron beam have been studied. It has been shown that spectra of radioluminescence arisen from the effect of an electron beam and spectrum of the following explosive luminescence coincide. The spectrum of pre-explosive dlow has been found to be of luminescent nature. Linear spectrum of explosion products has been registered. It can be associated with molecular nitrogen luminescence.
NTREM, PARDUBICE, 2004 page 404-408

THE EXPLOSION PARAMETERS OF BENZOYL AND CYCLOHEXANONE PEROXIDES

N.I. Akinin*, S.V. Arinina*,G.D. Kozak*, I.N. Ponomarev**

* Mendeleev University of Chemical Technology 125047, Miusskaja sq. 9, Moscow, Russia
** Joint-stock company "POLION-P" 125047, Miusskaja sq. 9, Moscow, Russia

Abstract:
The ultimate objective of the work was to investigate the ability to heat explosion, burning and detonation of some organic peroxides. The main attention was paid in previous work to investigation ofcumene hydroperoxide (CH). The properties ofbenzoyl peroxide (BP), and cyclohexanone peroxide (CHP) were collected and analyzed in this work. The explanation of the investigation results focused on identifying the most probable occurring chemical reactions at decomposition, heat explosion, burning and on reaction thermochemistry data. The data of investigation in couple with literature materials characterize net cyclohexanone peroxide, cumene hydroperoxide, and benzoyl peroxide as weak explosive, which are able to burning, low velocity detonation, and heat explosion. The results of investigation update the information concerning to explosion characteristics of CHP, CH, and BP and they could be used to achieve accident prevention goal on the plant facilities at its production, processing treatment, and transportation.
NTREM, PARDUBICE, 2004 page 409-418

AN EXPERIMENTAL CHECKING OF A DIVACANCY MODEL OF INICIATING HEAVY METAL AZIDES[1]

E.D. Aluker*, A.G. Krechetov*, A.Yu. Mitrofanov*, B.G. Loboiko, D.R. Nurmuhametov* and E.V Tupitsin***

* Kemerovo State University, 650043, Kemerovo, Russia
** Russian Federal Nuclear Center, All-Russia Research Institute of Technical Physics (RFNC-VNIITF) 456770, PO Box 245, Snezhinsk, Chelyabinsk region, Russia

Abstract:
Main results are adduced of an experimental checking of a divacancy model ofiniciating heavy metal azides. The analysis result shows that a divacancy model ofiniciating heavy metal azides quantitatively do agree with available theoretical data.
NTREM, PARDUBICE, 2004 page 419-423

COMPARATIVE CHARACTERISTICS OF TWO ISOMERIC EXPLOSIVES: 4-NITRO-5-NITRIMINO-1H-1,2,4-TRIAZOLE AND 3-NITRO-5-NITRIMINO-1,4H-1,2,4-TRIAZOLE

A.M. Astachov, V.A. Revenko and E.S. Buka
Siberian State Technological University, Prosp. Mira 82, 660049 Krasnoyarsk, Russia
Abstract:
The comparative estimation of properties of two isomeric nitroderivatives of 1,2,4-triazole - 4-nitro-5-nitrimino-1H-1,2,4-triazole and 3-nitro-5-nitrimino-1,4H-1,2,4-triazole, is realized. In contrast to the C-nitrocompound, the N-nitrocompound has higher heat of formation, and as a consequence, the higher explosive characteristics. On the other hand, N-nitrocompound has lower thermal stability and higher impact sensitivity in comparison with C-nitrocompound.
NTREM, PARDUBICE, 2004 page 424-432

APPLICATION OF TLC FOR AN ANALYSIS OF INITIATING EXPLOSIVES

J. Błądek, R. Kowalczyk and S. Cudziło
Institute of Chemistry, Military University of Technology, Kaliskiego 2, 00–908 Warsaw, PL
Abstract:
Instrumental TLC was used for analyses of initiating explosives (IHE). A chromatographic system suitable for analyte separation and method of densitometric determination of some IHE complexes with ditizone were proposed. A linear dependence of densitometric peak areas A on the analyte mass c in the chromatographic band was obtained (Hg: A =33202c —1406 and Pb: A = 42643c - 83). A limit detection (Hg: 7.15 and Pb: 1.25 ng in the chromatographic band) and maximal range of linear measurements (Hg: 120 and Pb: 20 ng) was determined. The method developed was used to analyze chosen IHE in electrolytes.
NTREM, PARDUBICE, 2004 page 433-436

APPLICATION OF CARBONACEOUS PRODUCTS OF HALOGENOCARBONS REDUCTION FOR SOLID PHASE EXTRACTION

J. Błądek, A. Arciszewska, S. Cudziło and W. Kiciński
Institute of Chemistry, Military University of Technology, Kaliskiego 2, 00–908 Warsaw, PL
Abstract:
The possibility of application of carbon materials sensitized in self-propagating heat waves for solid phase extraction (SPE) is presented. Extraction cartridges with the materials were prepared, and samples of water contaminated with pesticides (PDs) and polycyclic aromatic hydrocarbons (PAHs) were analyzed. Modern TLC equipment was used for analyses. Chromatographic systems and analytical parameters of PDs and PAHs were defined and these results were used to determine some retention and elution characteristics of the tested materials. Recovery and measuring errors were estimated (the recovery equaled ca. 50 % and the SD was below 6 %). It was shown that some of the examined materials can be applied as adsorbents for SPE. They are especially good for extraction of analytes with comparatively high polarity.
NTREM, PARDUBICE, 2004 page 437-442

THE EXAMINATION OF CHOSEN BALLISTIC PARAMETERS OF IGNITER CHARGE $BKNO_3$ FOR IGNITERS OF SOLID PROPELLANT ROCKET MOTORS

M. Cieślikowska, M. Moskalewicz and T. Wolszakiewicz
Institute of Organic Industrial Chemistry, Annopol 6, 03 - 236 Warsaw, Poland

Abstract
The preliminary results of pyrostatic investigations of ignition tablets BKNO3 were prestented. The investigations were performed in especially designed for this purpose rocket engine with established constant loading density. The time of burning and dynamics of process were estimated.
NTREM, PARDUBICE, 2004 page 443-450

SYNTHESIS AND SOME PROPERTIES OF BU-NENA

K. Dudek*, P. Mareček*, J. Skládal* and Z. Jalový**
* Explosia a.s. Research Institute of Industrial Chemistry (VÚPCH), CZ-532 17, Pardubice-Semtín, Czech Republic
** Department of Theory and Technology of Explosives, University of Pardubice, CZ-532 10 Pardubice, Czech Republic

Abstract:
Butyl-NENA was synthesized by two-step reaction in laboratory and pilot plant scale. The product was identified by means of ^{1}H, ^{15}NNMR spectra, IR spectra and elementary analysis. Purity of the sample was determined by HPLC. Evaluated parameters were sensitivity to impact, DTA analysis and acidity ofBu-NENA. The results, especially with regard to utilization of Bu-NENA as a component of propellants and explosives, are discussed.
NTREM, PARDUBICE, 2004 page 451-458

ANALYSIS AFTER COMBUSTION OF PROPELLANTS

A. Eisner*, M. Adam*, K. Ventura*, V. Ježová* and J. Skládal**
* Department of Analytical Chemistry, Faculty of Chemical - Technology, University of Pardubice, Nám. Čs. Legií 565, Pardubice 532 10, CZ
** Research Institute of Industrial Chemistry, Explosia a.s., Pardubice - Semtín 532 17, CZ

Abstract:
The aim of this study is an identification of products after combustion of smokeless powders and solid propellants. In first a sample of smokeless powder was burnt on the clean sand. Than an isolation of compounds from this sand was tried. The accelerated solvent extraction and ultrasonication were used for the isolation of these compounds. Gas chromatography GC 17A with mass spectrometry detector QP505A was used for an identification of compounds.
NTREM, PARDUBICE, 2004 page 459-462

DINITROBIURET AND ITS SALTS

J. Geith, K. Karaghiosoff, T.M. Klapötke, P. Mayer and J. Weigand
Department of Chemistry and Biochemistry, University of Munich, Butenandtstr. 5-13 (D), D-81377 Munich (Germany)

Abstract:
The work summarizes knowledge about Dinitrobiuret (DNB) - about its important explosives characteristics and parameters. It is focused on preparation, determination of molecular structures and the results of IR-Raman and multinuclear NMR spectroscopic investigations.
NTREM, PARDUBICE, 2004 page 463-466

EFFECTS ON ENFRGETIC MATERIALS PROCESSED WITH POWER ULTRASOUND

V.I. Grozev*, R.H. Ganev and Z. S. Grozeva*****

* Konstantin Preslavsky University of Shumen, University str.1 15, 9712 Shumen, Bulgaria (BG)
** University of Chemical Tachnology and Metallurgy, Kliment Ohridski blvd. 8, 1756 Sofia, Bulgaria (BG)
*** Konstantin Preslavsky University of Shumen, University str. 115, 9712 Shumen, Bulgaria (BG)

Abstract:

We present experimental results derived by the effect of a high power ultrasound on melts of explosives and solutions of propellants. An effect of increase of the speed of formation of crystallisation centers have been identified for 2,4,6-trinitrotoluene and mixtures on its base. We investigated the kinetics of destruction of nitrocellulose in ultrasound field in solution of gunpowders.

NTREM, PARDUBICE, 2004 page 467-471

STUDY ON RING CLEAVAGE AND ADDUCTIVE PROPERTY OF 2-(DINITROMETHYLENE)-4,5-IMIDAZOLIDINEDIONE

Cai Hua-Qiang, Shu Yuan-Jie, Huang Hui and Cheng Bi-Bo

Institute of Chemical Materials, China Academy of Engineering Physics, 621900, Mianyang, China

Abstract:

Ring cleavage of 2-(dinitromethylene)-4,5-imidazolidinedione (1) was achieved by methanol for the first time and the product was 1,1-diamino-2,2-dinitroethylene (FOX-7). 2, the first adduct of1, was synthesized by the reaction of1 with methanol in certain conditions and its structure was characterized. Physical and chemical properties of the adduct were studied. Parabanic acid was synthesized by decomposition of 1 in methanol, losing nitrogen oxides and carbon oxides.

NTREM, PARDUBICE, 2004 page 472-478

AGEING INFLUENCE ON STABILITY AND SENSITIVITY OF PETN EXPLOSIVES

M. Chovancová, P. Očko, M. Lazar and A. Pechová

VTSÚ (Military Technical and Testing Institute) Zahorie, 905 24 Senica, SK

Abstract:

In this paper the PETN explosives stability and sensitivity are investigated during their artificial ageing. It was observed their stability was not changed, but sensitivity was changed after ageing. The biggest change was recorded in sensitivity to electrostatic discharge offlegmatizedPETN.

NTREM, PARDUBICE, 2004 page 479-486

EXPLOSIVE TYPE SELECTION WITH RESPECT TO THE VENTILATION CYCLE DURATION

B. Janković, D. Vrkljan and Z. Ester

Faculty of Mining, Geology and Petroleum Engineering, Pierottijeva 6, 10-000 Zagreb, Croatia

Abstract:

Extensive measurements of the ambient air quality have been conducted in the past years during excavation of road tunnels situated on the mountainous sections of the future Croatian highway Zagreb - Split. The objective of these measurements was to estimate the worker exposure to toxic gases. Since conventional mining methods have been used for excavation of the tunnels (drilling and blasting), as well as various types of explosives and initial systems, the impact on the workplace environment by toxic gases produced from blasting was also examined. In order to reduce the amount of toxicants in the workplace atmosphere, the field method for selection of the most appropriate types of explosives in the blast charge was developed.

NTREM, PARDUBICE, 2004 page 487-492

DISSOLVER VER. 1.1 HELPS CENTRAL MINING RESCUE STATION

B. Janovský
Dept. of Theory and Technology of Explosives, University of Pardubice, 532 10 Pardubice, CZ

Abstract:
This paper introduces new software package DisSolver v. 1.1, which was developed under the contract between Czech Mining Authority and University of Pardubice. The package consists of three individual codes - "Výbuchový trojúhelník", "Následky" and "Vodní zátky". Code "Výbuchový trojúhelník" solves the problems with explosibily of atmosphere inside the coal mines. Code "Následky" enables the user to calculate the consequences of accidental leaks of natural gas and crude oil during the drilling. Code "Vodní zátky" solves the mathematical model of the water column movement in the gallery as the method of the explosion-proof closing of the seat of fire in the coal mines.
NTREM, PARDUBICE, 2004 page 493-504

EXPANSION OF METALLIC TUBES DRIVEN BY HEAD-ON GRAZING DETONATION

Chen Jun and Sun Chengwei
Laboratory for Shock Wave and Detonation Research, Southwest Institute of Fluid, CAEP, POBox 919-103, Mian Yang, Sichuan 621900, P.R.China

Abstract:
Since the pressure gradient abruptly increase in the detonation products undergoing a head-on collision of two detonation waves propagating in the cylindrical charge embedded in a metallic tube, the movement of tube wall driven by which will be of particular pattern. The data of expansion, deformation and fracture of the tube are obtained in the experiments with diagnostics of pulsed x-ray shadowgraphy and highspeed photography. A 2-D elastic plastic hydrodynamic Lagrangian code TTD2C has been compiled during this work and succeeded in simulating the head-on collision of two detonation waves and the resulting products flow, also the expansion process of metallic tubes driven by it. The calculated and measured results agree well with each other. The result shows that the fracture time advanced because of the head-on collision.
NTREM, PARDUBICE, 2004 page 505-511

NONAERATIONS SENSIBILIZATION OF EMULSIVE EXPLOSIVES

I.L. Kovalenko*, V.P. Kuprin and A.V. Kuprin*****
* Faculty of inorganic chemistry, Ukrainian state university of chemical technology, Gagarin av. 8,49005 Dnepropetrovsk, UA
** Faculty of physical chemistry, Ukrainian state university of chemical technology, Gagarin av. 8,49005 Dnepropetrovsk, UA
*** ECCOM Ltd, Serova str. 15/26,49070 Dnepropetrovsk, UA

Abstract:
The opportunity of reception bull water-tight (4100-4400 κJ/kg) emulsive explosives such as "water in oil" is shown on the basis of solution of nitrocalcites and ammonium at the expense of sensibilization by the solid high-energy additives. The sensibilization of emulsive explosives is carried out at the expense of the addition of powders of metals and alloys with high hardness, melting point and capacity to react with light-end products of detonating. The responsive efficient explosive is prepared out without padding aeration, introducing of microspheres and explosive reagents.
NTREM, PARDUBICE, 2004 page 512-515

THE CONDENSED EXPLOSIVE SYSTEMS CAPABLE OF PROPAGATING DETONATION IN THE SPIN-PULSATING REGIME

G.D. Kozak* and Z. Lin**

* Mendeleev University of Chemical Technology Miusskaya Sq.9, Moscow, 125190

** Beijing Institute of Technology, P O Box 327, Beijing 100081, China

Abstract:

Quite distinct inhomogeneity of the detonation front was found earlier at detonation of cast charges TNT/RDX and TNT/PETN. The ultimate objective of this work is to extend the number of explosive systems capable of propagating detonation in the spin-pulsating regime and to generalize the results. Cast TNT/DINA, TNT/TETRYL DNT/PETN and pressed HMX/paraffin charges were investigated. Systems, detonating with low (1~3 MHz) frequency spin pulsation at some content of sensitizer (Cs), have approximately the same calculated detonation parameters: DJ ≈ 7.3-7.4 km/s, Q_V≈ 5.4 MJ/kg. The compositions TNTDINA with C_S>25%, which detonate without spin pulsation, have calculated values Q_V and DJ higher than that named above. Q_V and DJ of itself DINA sufficiently higher than 5.4 MJ/kg and 7.3~7.4 km/s, correspondingly, and spin pulsation at detonation of charges of liquid Dina were not observed.

NTREM, PARDUBICE, 2004 page 516-523

DETONATION ABILITY OF SOLUTIONS OF AROMATIC NITROCOMPOUNDS IN NITRIC ACID

G.D. Kozak, V.M. Raikova and V.V. Potapov

Mendeleev University of Chemical Technology 125047, Miusskaja sq. 9, Moscow, Russia

Abstract:

The ultimate objective of our work was to measure the failure detonation diameters of solutions ofnitro derivative of toluene: TNT, DNT and MNT, and ofnitro derivative of benzene: TNB, DNB andMNB in strong nitric acid at oxygen balance A=0%. They were measured by means of technique of parallel-plate cells. The cells were glued from glass photo plates, each of them had the constant thickness (1.1-1.4 mm). The clearance of cells was made by means of placing teflone sheets between sides of glass plates Equivalent failure diameter of detonation of the solution of TNT and TNB was df=0.10 mm, of DNT and DNB - df=0.18 and 0.15 mm, and of MNT and MNB - df=0.6 and 0.2 mm, correspondingly. Simultaneously the detonation parameters of the solutions investigated were calculated by means ofSD computer code at experimentally measured densities of solutions. Distinction of df values was explained by discrepancy of its calculated detonation parameters.

NTREM, PARDUBICE, 2004 page 524-529

FAULT TREE ANALYSIS IN THE PROCESS SAFETY INCIDENT INVESTIGATION

R. Kuracina, B. Janovský and M. Ferjenčík

Department of Theory and Technology of Explosives, University of Pardubice, Czech Republic

Abstract:

This contribution is focused on methods for incidents investigation and its application in chemical industry. It contains a literal retrieval focused on basic principles of incident investigation and in practice section using one of the basic investigation techniques -Fault Tree Analysis. System evaluation of gelatination of nitrocellulose oriented to fire in object is the result of this work. "Minimal cut sets" (MCS) was obtained from the basic events probability of the constructed fault tree. Probability of incidents was then determined from MCS causes and corrective actions were recommended. In final part of this contribution, benefits and deficiencies of this systematic incident investigation was compared with traditional investigation with commission.

NTREM, PARDUBICE, 2004 page 230-540

INTERNAL BALLISTIC ANALYSIS OF THE 20 × 102 CARTRIDGE

K. Leinweber and J. Petržílek
Explosia a.s., 532 17, Pardubice - Semtín, CZ

Abstract
Results obtained by two different methods of pressure measurement are discussed. Maximum pressures were measured simultaneously in the cartridge of medium calibre weapon 20 x 102 mm by copper crusher and piezo transducer. Results obtained by different methods were correlated and influence of testing temperature was discussed.
NTREM, PARDUBICE, 2004 page 541-545

UNSATURATED POLYESTER INHIBITION SYSTEM FOR DOUBLE BASE PROPELLANTS

M. Lipiński, K. Lipińska, B. Florczak and W. Witkowski
Institute of Industrial Organic Chemistry, 6 Annopol St., 03-236 Warszawa, Poland

Abstract:
Inhibitors are applied to those surfaces of the propellant grain where burning is to be prevented. We investigated inhibition system for double base propellants based on unsaturated polyesters resins. Measurements of the amount of nitroglycerine that migrates into the chosen inhibitors were done using a "sandwich" test. Double base propellant grains were inhibited by a casting technique and statically fired in rocket motor. The nature of P-t profiles suggested that it is potential inhibition system for double base propellants.
NTREM, PARDUBICE, 2004 page 546-552

SYNTHESIS OF DI(1H-TETRAZOLE-5-YL)AMINE (BTA)

P. Mareček*, K. Dudek*and F. Liška**
* Explosia a.s. Research Institute of Industrial Chemistry (VÚPCH), CZ-532 17, Pardubice-Semtín, Czech Republic
** Institute of Chemical Technology, Faculty of Chemical Technology, Department of Organic Chemistry, CZ-166 28 Prague, Czech Republic

Abstract:
New method of synthesis of di(1H-tetrazole-5-yl)amine is described in the paper. Di(1H-tetrazole-5-yl)amine was synthetized by reaction of sodium azide with sodium dicyanamide in water under presence of zinc chloride as catalyst. This new method eliminates disadvantages of other alternative methods, such as for example: work with expensive and toxic metals, work with excess of volatile and toxic azoimide or work with organic solvents. This synthesis is very simple, safe and provides a good yield.
NTREM, PARDUBICE, 2004 page 553-556

CHANGES OF DYNAMIC MECHANIC PROPERTIES OF DOUBLE BASED ROCKET PROPELLANT DURING ARTIFICIAL AGEING

S. Matečić Mušanić, M. Sućeska, M. Rajić Linarić, B. Sanko and R. Čuljak
Brodarski institut–Marine Research & Special Technologies Av. V. Holjevca 20, 10020 Zagreb, Croatia

Abstract:

Double based rocket propellants are subjected to a chemical ageing, as well as ageing due to physical and physical-chemical processes (migration of low molecular constituents: plasticizers, blasting oil, burning catalysts, degradation of molar mass, etc.). The ageing has significant influence on their relevant properties, including mechanical properties such as tensile strength, storage modulus, loss modulus, tan delta, and temperature of glass transition, etc.
During use these changes can result in dangerous failures, such as rocket motor explosion. Therefore, it is necessary that after some time, temperature, and stress conditions, relevant properties of the propellants are still in the range of acceptable tolerance.
In this work we have studied changes of dynamic mechanic properties (loss modulus, storage modulus, tan delta, etc.) with the artificial ageing at higher temperature (90°C). The results obtained have shown that dynamic mechanical parameters change significantly after ~40 days of ageing. It was found put that the most sensitive parameters on the ageing process are: storage modulus at the room temperature, glass transition temperature, width of peak on loss modulus curve in the glass transition region, and tan δ at the glass transition region.
NTREM, PARDUBICE, 2004 page 557-570

APPLICATION OF SHEET EXPLOSIVE FOR METAL HARDENING

P. Nesvadba
Explosia a.s., Research Institute of Industrial Chemistry 532 17 Pardubice -Semtín, Czech Republic
Abstract:
This article contains a brief information on application of sheet charges for explosive hardening of metals. The paper defines basic requirements for the properties of the explosives used for explosive metal hardening, resulting from practical applications. Atthe same time the findings are given here obtained at application of the explosive at hardening ofHadfield steel.
NTREM, PARDUBICE, 2004 page 571-575

INFLUENCE OF INSENSITIVE ADDITIVES ON DETONATION PARAMETERS OF PBX

A. Orzechowski*, D. Powała*, A. Maranda and J. Nowaczewski****
* Institute of Industrial Organic Chemistry, 6 Annopol St, 03-236 Warszawa, PL ** Military University of Technology, 2 Kaliskiego St, 00-908 Warszawa 49, PL
Abstract:
Plastic bonded explosives (PBX) are known as explosives which possess high energy, thermal stability, low insensitivity and good mechanical properties. We investigated plastic explosive based on hexogen. As an additive we used NTO. We researched influence of NTO additives on detonation parameters of plastic explosives. This additive generated the decrease of sensitivity without significant worsening detonation parameters.
NTREM, PARDUBICE, 2004 page 576-583

AN UNDERWATER TEST FOR LWC EMULSION EXPLOSIVES

J. Paszula*, A. Maranda*, B. Gołąbek and J. Kasperski****
* Military University of Technology, 00-908 Warszawa, ul. Kaliskiego 2, Poland ** Blastexpol, Duninów, Poland
Abstract:
In the paper results of some experimental investigations of underwater shock waves parameters generated by explosion of TNT and water-in-oil emulsion explosives are presented. In experiments, the overpressure history in transient shock wave generated by explosion of investigated explosive charges was measured. Moreover numerical evaluation of shock waves energy and bubble energy released during explosion is performed. These calculated parameters could be used as parameters of explosive performance. Comparison of the explosion energy of various kinds of explosives is

performed. An influence of aluminium powder on energy released is discussed..
NTREM, PARDUBICE, 2004 page 584-590

PREDICTION OF THERMODYNAMIC CONDITIONS FOR NITROESTER VAPOR CONDENSATION ON THE SURFACES OF PROCESS APPARATUS DURING THE PRODUCTION OF ENERGETIC MATERIALS

D.V. Pleshakov and Y.M. Lotmentsev
Mendeleyev University , Department of Chemical Engineering, 125047 Miusskaya pl.9, Moscow, Russia

Abstract:
A calculation procedure has been developed for finding thermodynamic conditions under which nitroglycerine, diethylene glycol dinitrate, and triethylene glycol dinitrate vapors are condensed on the surfaces of process apparatus during the production of energetic materials. Temperature – (plasticizer content in dry air) diagrams have been calculated and mapped. The diagrams allow one to estimate the condensation temperature of supersaturated nitroester vapor and to calculate the condensate weight. A procedure has been proposed for measuring the partial saturated vapor pressure of a plasticizer under the production conditions.
NTREM, PARDUBICE, 2004 page 591-599

STUDY OF ELECTRON DENSITY OF MOLECULES, INTERMOLECULAR FORCES AND IMPACT SENSITIVITY OF EXPLOSIVES

Miroslav Pospíšil* and Pavel Vávra**
* Charles University, Faculty of Mathematics and Physics, Ke Karlovu 3, 12116 Prague 2, Czech Republic
** University of Pardubice, Department of Theory and Technology of Explosives, Studentská 95, 53210 Pardubice, Czech Republic

Abstract:
The electron densities for the selective set of twenty explosives with composition C-H-N-O were calculated (i) for individual molecules and (ii) for molecules placed in crystal cell. Indirect linearity of absolute difference of charges for bonds C-NO_2, N-NO_2 and O-NO2 versus the length of the bond was founded in both cases. The influence ofnon-covalent hydrogen bonds for distinctly decreasing of the impact sensitivity was confirmed. On the base of results from experimental methods such as the impact sensitivity and theoretical methods such as molecular mechanics and molecular density calculations for selected set of twenty explosives the possibilities of prediction for impact sensitivity of new energetic materials are discussed.
NTREM, PARDUBICE, 2004 page 600-605

SPHERICAL NITROGUANIDINE AS COMPONENT OF HIGH EXPLOSIVES

D. Powała*, A. Orzechowski*, A. Maranda and J. Nowaczewski****
* Institute of Industrial Organic Chemistry, 6 Annopol St, 03-236 Warszawa, PL ** Military University of Technology, 2 Kaliskiego St, 00-908 Warszawa 49, PL

Abstract:
Researches on nitroguanidine (NGU) crystallization were conducted in order to obtain spherical crystals. We investigated plastic bonded explosive based on hexogen with NGU as an additive. Nitroguanidine, as a component of PBX generated the decrease of sensitivity to mechanical stress without worsening other parameters.
NTREM, PARDUBICE, 2004 page 606-613

THE CHEMICAL KINETIC AT DETONATION OF AROMATIC NITROCOMPOUNDS - NITRIC ACID MIXTURES

V.M. Raikova and E.A. Likholatov
Mendeleev University of Chemical Technology, Miusskaya sq. 9, Moscow A-47, Russia

Adstract:
Detonation failure diameter df of mixtures of six aromatic Nitrocompounds with nitric acid has been examined in the framework of A.Dremin theory. Shock and detonation parameters as well as characteristics (P3, T3 and τ3) of the reaction zone to determine reinitiation of detonation wave at low diameters of the charge were calculated by means of SGKR computer package. According to our calculations maximum of T_3 values was fixed at the concentrations of nitric acid corresponding to the minimum of df. Effective values of kinetic parameters of reaction between nitric acid and Nitrocompounds are defined.
NTREM, PARDUBICE, 2004 page 614-620

INITIAL STAGE DECOMPOSITION KINETICS OF NITROCELLULOSE PROPELLANT

M. Rajić Linarić, M. Sućeska, S. Matečić Mušanić and R. Čuljak
Brodarski institut–Marine Research & Special Technologies Av. V. Holjevca 20, 10020 Zagreb, Croatia

Abstract:
A thermal decomposition reaction in nitrocellulose, which is the basic component of homogeneous propellants, limits the safe use and safe storage time of propellants. Under certain conditions the decomposition may lead to the well-known phenomenon of self-ignition.
In order to be able predict the shelf-life and thermal hazard potential of propellants it is of vital importance to know a true decomposition mechanism and true vales of kinetic constants.
In this work we have studied decomposition kinetics of nitrocellulose propellant during the initial decomposition stage (up to 2 % mass loss) at elevated temperatures ranging from 80 to 100 °C. The kinetic results were derived from sample mass loss-time/temperature. It was found out that the activation energy for this decomposition stage equals 123.4 kJ/mol, and pre-exponential factor $1.78\text{-}10^6$ 1/s. Also, it was found out, on the basis of the kinetic data obtained, that the reaction rate accelerating factor changes with temperature -from ~3 at 90-100 °C temperature range to about 5.5 at the room temperatures.
NTREM, PARDUBICE, 2004 page 621-629

DETERMINATION OF THE RELATIVE DENSITY OF MOLTEN EXPLOSIVES

Fritz van Rooyen
National Institute for Explosives Technology (NIXT) South Africa PO Box 32544, Glenstantia 0010, Pretoria, Republic of South Africa

Abstract:
The Archimedes principle was used for the determination of the relative density of molten TNT. This method proves to be practical, easily conducted and quick, providing reliable results with high precision and sensitivity.
NTREM, PARDUBICE, 2004 page 630-635

COMBUSTION OF DINITRAMIDE SALTS

V.P. Sinditskii, A.I. Levshenkov, V.Yu. Egorshev and V.V. Serushkin

Mendeleev University of Chemical Technology, 9 Miusskaya Square, 125047, Moscow, Russia
Abstract:
Burn rate studies have been carried out on dinitramide salts of common formula of L nHN(NO_2)2, (where n = 1 or 2; L = methylamine, trimethylamine, tret-butylamine, tetramethylammonuim, urea, guanidine, aminoguanidine, triaminoguanidine, ethanolamine, diethanolamine, ethylenediamine, hexamethylenediamine, aniline, 3-nitroaniline, 2-toluidine, benzylamine, phenylhydrazine, morpholine, piperazine, pyridine, 3,5-dimethylpyridine, and 5-aminotetrazole) as well as lithium and barium salts of dinitramide. Most of the salts exhibit either combustion instability (like ADN) or a transition region on their $r_b(p)$ curves. The occurrence of this region depends upon the fuel reactivity and, largely, the surface temperature which is assumed to be dissociation one and dependent on the amine basicity. To disclose combustion mechanism, flame structure of hexamethylenediamine dinitramide (GMDADN) has been investigated with tungsten-rhenium microthermocouples. Besides, burn rate study of GMDADN within a wide initial temperature interval allowed the burning rate temperature sensitivity to be evaluated.
NTREM, PARDUBICE, 2004 page 636-645

DETERMINATION OF CHEMICAL STABILITY OF GUNPOWDERS BY QUALITATIVE AND QUANTITATIVE METHODS

R. Smileski, O. Popovski and J. Naumoski
Military Academy "General Mihailo Apostolski" Skopje, Republic of Macedonia
Abstract:
This work presents the results from the analyses made on monobasic gunpowder, which consists of two types of stabilizers (diphenylamine and centralit I) with total mass of representation of about 1,3%.
The content of the residual stabilizer of gunpowder treated at different temperature and at different length of time was determined by using two quantitative methods.. By processing and comparing the results gained at raised temperature an attempt was made to foresee the time of stability of the gunpowder in normal conditions of storing. As quantitative methods in this case The Hansen test and liquid chromatography (HPLC) were applied According to the first method the gunpowder was treated at 110 °C in the period from 0 to 72 h, and the results were validated by using pH - meter. The second method was used to determine the content of the residual stabilizer at the same gunpowder treated at 110°C as long as the content of the active stabilized does not go below 50% m/mfrom the starting one.
NTREM, PARDUBICE, 2004 page 646-652

DETERMINATION OF EXPLOSIVE PROPERTIES

R. Špásová
Explosia a. s.,Research Institute for Industrial Chemistry, Safety Engineering Laboratory, 532 17 Pardubice-Semtín,CZ
Abstract:
This paper informs about testing of explosiveness of chemical substances according Ministry of Environment Decree which becomes valid to the date of entering the Treaty of Accession of Czech Republic to Europen Union into force.
NTREM, PARDUBICE, 2004 page 653-658

GEMINAL DINITROCOMPOUNDS THERMAL DECOMPOSITION UNDER NON-ISOTHERMAL CONDITIONS

R.S. Stepanov, L.A. Kruglyakova and A.M. Astachov

Siberian State Technological University 660049, Krasnoyarsk, prosp. Mira 82, Russia
Abstract:
Depending on geminal trinitrocompounds structure, their thermal decomposition proceeds in one or two stages. It is a complex process that includes evaporation, destruction, secondary oxidation-reduction reactions, and autocatalysis. It is shown that thermal sensitivity is tied with temperature of initial decomposition. The steric effect of α-substituent at geminal dinitrogroup significantly influences both decomposition rate constant and decomposition's characteristic temperature. Corresponding quantitative correlations confirm it.
NTREM, PARDUBICE, 2004 page 659-666

DETONATION PERFORMANCES OF LOW-SENSITIVITY NTO/HMX EXPLOSIVES

W. A. Trzciński and L. Szymańczyk
Military University of Technology, Kaliskiego 2, 00 908 Warsaw, Poland
Abstract:
Detonating performances of new explosive compositions containing NTO andHMX are investigated in this work. Detonation velocity, pressure and energy of the mixtures tested and acceleration ability and equation of state of their detonation products are determined. Shock and impact sensitivity is evaluated in the gap test and heavy hammer test. The compositions investigated can be considered as a suitable insensitive explosive to replace TNT/RDX mixtures in munitions applications.
NTREM, PARDUBICE, 2004 page 667-675

TRACE ANALYSIS OF EXPLOSIVES BY LC-MSD TECHNIQUE

R. Varga*, P. Ulbrich, M. Kološvári** and M. Fuknová****
* Department of Theory and Technology of Explosives, University of Pardubice, 532 10 Pardubice, Czech Republic
** Institute of Forensic Science of the Slovak Police Corps, Sklabinská 1, Bratislava 812 72, Slovak Republic
Abstract:
The aim of this work is the determination ofLOD of explosive compounds using Agilent 1100 series LS-MSD system with the atmospheric pressure chemical ionization (APCI) source. At the analysis of explosive compounds LC-MSD with IONSCAN M 400 (Barringer Inc.), a detector of explosives and drugs, and with the gas chromatography with electron capture detector (agilent Technologies) were compared.
NTREM, PARDUBICE, 2004 page 676-686

LIFE-CYCLE-ANALYSIS AND "GREEN" ENERGETIC MATERIALS

J. Vávra* and P. Vávra **
* Department of Economy and Management of Chemical and Food Industry, Faculty of Chemical Technology, University of Pardubice, 53210 Pardubice, Czech Republic
** Department of Theory and Technology of Explosives, Faculty of Chemical Technology, University of Pardubice, 53210 Pardubice, Czech Republic
Abstract:
This paper mentioned the main requirements on "green" energetic materials and the priorities in specific programs in R&D. In this connection with these new requirements are principles of Life-Cycle-Analysis (LCA) and Life-Cycle-Costs (LCC) applicated. Possible use of these methods for costs reduction of new GEM during whole GEM's lifetime is discussed.
NTREM, PARDUBICE, 2004 page 687-693

MODERN PROPELANTS FOR 30 MM AMMUNITION APPLICATIONS

L. Velehradský, J. Petržílek and V. Puš
Explosia a.s., Research Institute for Industrial Chemistry (VÚPCH), CZ-532 17, Pardubice - Semtín, Czech Republic

Abstract:
This short survey is to provide some important information about new trends in development of propellants for existing modern weapon systems, or, propellants for ammunition for elder weapon systems with improved performance
NTREM, PARDUBICE, 2004 page 694-698

DIRECT MONTE - CARLO SIMULATION OF DETONATION PROCESS IN A GAS

Z.A. Walenta*, A. Teodorczyk and W. Witkowski*****
* Institute of Fundamental Technological Research, Polish Academy of Sciences Swietokrzyska 21, 00-049 Warszawa, Poland
** Institute of Heat Engineering, Warsaw University of Technology Nowowiejska 25, 00-665 Warszawa, Poland
*** Institute of Industrial Organic Chemistry Annopol 6, 03-236 Warszawa, Poland

Abstract:
The research on gaseous detonation has recently become a very important issue because of increasing importance of gaseous fuels. We propose to use the Direct Monte - Carlo Simulation technique, which is a very powerful tool for solving complex flow problems. We propose a very simple model of a molecular collision, which makes it possible to increase the thermal energy of a gas, which is similar to the processes in the flame. We show then, that this model can produce the wave, which has the features characteristic for a detonation wave.
NTREM, PARDUBICE, 2004 page 699-703

SYNTHESIS OF 4,6-DINITROBENZOFUROXAN

V.L. Zbarsky, D. M Stepashkow and N.V. Yudin
Mendeleev University of Chemical Technology, 9 Miusskaya Square, 125047, Moscow, Russia

Abstract:
Problems connected with nitration of benzofuroxan are of specific interest since potassium salt of dinitrobenzofuroxan is considered as promising ecologically pure initiating explosive. In this connection a study has bin performed on nitration of benzofuruxan and its mononitroderivatives in nitric and sulfuric- nitric acid mediums. The main reaction products formed in the reaction have been identified.
NTREM, PARDUBICE, 2004 page 704-707

APPLICATION POSSIBILITIES OF POLAROGRAPHY IN STUDIES OF CHEMICAL MICRO-MECHANISM OF INITIATION OF POLYNITRO ARENES

S. Zeman and E. Zemanová
Department of Theory & Technology of Explosives, University of Pardubice,CZ-532 10 Pardubice, Czech Republic

Abstract
The half-wave potentials, E1/2, *of twenty four polynitro arenes have been determined in aqueous*

medium buffered at pH 7, the final concentrations of their solutions being 0.5x10–^{4} M and 0.5x10–^{5} M. The ^{13}C NMR chemical shifts of carbon atoms carrying the most reactive nitro groups have been used for specification of the primarily reduced nitro group in the molecule. The found logical relationships between the $E1/_2$ *values and squares of detonation velocity are of the type of the modified Evans-Polanyi–Semenov equation for energetic materials. It has been stated that the strong dependence of E1 values on the conditions and way of realisation of the polarographic measurements considerably restrict the application of this method to studies of micro-mechanism of initiation of organic energetic materials.*
NTREM, PARDUBICE, 2004 page 708-716

IN SITU MEASUREMENT OF VELOCITY OF DETONATION AND COMPARISON OF HEAVY ANFO PRODUCED IN THE FIELD OF USAGE AND CARTRIDGE EXPLOSIVES

S. Žganec*, E. Zvonimir and M. Dobrilović****

* Minervo Ltd, Ljubljana, Slovenia

** Faculty of Mining, Geology and Petroleum Engineering, University of Zagreb, Croatia

Abstract:

This paper describes methods of measuring the velocity of detonation in bore holes loaded with different types of bulk explosive, such as heavy ANFO and cartridge explosives. The explosives are produced at the point of use with mobile equipment. The measurements of the velocity of detonation (VOD) involved bore holes with different diameters. On this basis the interdependence of the VOD and the bore-hole diameter was determined. The VOD measurements, with different blasting parameters, can be used for the selection of the best explosives to be produced at the site, taking into account the geological characteristics of the blasting rock.
NTREM, PARDUBICE, 2004 page 717